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FORM PTO-1390 U.S. DEPARTMENT OF CO	OMMERCE PATENT AND TRADEMARK OFFICE	ATTORNEY'S DOCKET NUMBER	
	ER 🗐 THE UNITED STATES	PVZ-006US	
DESIGNATED/ELECTED OFFICE (DO/EO/US)		U.S. APPLICATION NO. (If known, see 37 CFR 1.5)	
CONCERNING A FILING UNDER 35 U.S.C.371		00/01/459	
INTERNATIONAL APPLICATION PCT/SE00/00384	INTERNATIONAL FILING DATE 28 February 2000 (28.02.00)	PRIORITY DATE CLAIMED 4 4 2 26 February 1999 (26.02.99)	
TITLE OF INVENTION	CICN DAGED ON THE STREET	ODLITA WYDDOL ACE	
APPLICANT(S) FOR DO/EO/US	SIGN BASED ON THE STRUCTURE	OF LIA4HYDROLASE	
HAEGGSTRÖM, Jesper, Z et al.			
	States Designated/Elected Office (DO/EO/US	s) the following items and other information:	
1. E This is a FIRST submission	n of items concerning a filing under 35 U	J.S.C.371.	
2. This is a SECOND or SUI	BSEQUENT submission of items concer	ning a filing under 35 U.S.C. 371.	
	to promptly begin national examination p		
·	y the expiration of 19 months from the p		
	Application as filed (35 U.S.C. 371(c)(2)		
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	ne application was filed in the United Sta	tes Receiving Office (RO/US)	
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	; however, the time limit for making suc	h amendments has NOT avnirad	
d. A have not been made		is amendments has two rexpired.	
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8. An English language translation of the amendments to the claims under PCT Article 19 (35 U.S.C. 371(c)(3)). 9. An oath or declaration of the inventor(s) (35 U.S.C. 371(c)(4)). (unexecuted) (4 sheets)			
10. An English language translation of the annexes to the International Preliminary Examination Report under PCT Article 36 (35 U.S.C. 371(c)(5)).			
Items 11. to 16. below concern docu	ment(s) or information included:		
Di	Statement under 37 CFR 1.97 and 1.98.		
12. An assignment document included	for recording. A separate cover sheet in	compliance with 37 CFR 3.28 and 3.31 is	
13. 🗷 A FIRST preliminary ame	ndment. (12 sheets) (along with version	n of markings to show changes)	
☐ A SECOND or SUBSEQU	IENT preliminary amendment	a va marinago vo ono w enungeo)	
14. A substitute specification.	2111 prominary unionament.		
15. A change of power of attorney and/or address letter.			
16. Other items or information: Transmittal Letter (2 sheets in duplicate); International Application Published Under the PCT (with attached International Search Report) WO 00/50577 (156 sheets); PCT International Preliminary Examination Report (6 sheets); Certificate of Express Mailing (1 sheet); and return postcard receipt.			

JUUS heles to the su Z / AUG 2001 INTERNATIONAL APPLICATION NO. ATTORNEY'S DOCKET NO. U.S. APPLICATION NO. (if known, see 37 CFR 1.5) 09/91445 PCT/SE00/00384 PVZ-006US CALCULATIONS PTO USE ONLY 17. Ex The following fees are submitted: BASIC NATIONAL FEE (37 CFR 1.492 (a) (1) - (5)).(a/o November 1, 2000): Neither international preliminary examination fee (37 CFR 1.482) nor international search fee (37 CFR 1.445(a)(2)) paid to USPTO and International Search Report not prepared by the EPO or JPO......\$1000 International preliminary examination fee (37 CFR 1.482) not paid to USPTO but International Search Report prepared by the EPO or JPO\$860 International preliminary examination fee (37 CFR 1.482) not paid to USPTO but international search fee (37 CFR 1.455(a)(2)) paid to USPTO\$710 International preliminary examination fee paid to USPTO (37 CFR 1.482) but all claims did not satisfy provisions of PCT Article 33(1)-(4).....\$690 International preliminary examination fee paid to USPTO (37 CFR 1.482) and all claims satisfied provisions of PCT Article 33(1)-(4).....\$100 \$1,000.00 ENTER APPROPRIATE BASIC FEE AMOUNT = \$130.00 □ 30 Surcharge of \$130.00 for furnishing the oath or declaration later than 20 months from the earliest claimed priority date (37 CFR 1.492(e)). RATE NUMBER FILED NUMBER EXTRA **CLAIMS** X \$18.00 \$ 540.00 Total claims **50**-20 = 30 X \$80.00 \$ 160.00 Independent claims **5** -3 = MULTIPLE DEPENDENT CLAIM(S) (if applicable) +270.00\$ 270.00 \$2,100.00 TOTAL OF ABOVE CALCULATIONS = \$1,050.00 Applicant claims small entity status. See 37 CFR 1.27. The fees indicated above are reduced by 1/2. \$1,050.00 **SUBTOTAL** Processing fee of \$130.00 for furnishing the English translation later than \square 20 \square 30 months from the earliest claimed priority date (37 CFR 1.492(f)). TOTAL NATIONAL FEE = \$1,050.00 Fee for recording the enclosed assignment (37 CFR 1.21(h)). The assignment must be \$ accompanied by an appropriate cover sheet (37 CFR 3.28, 3.31). \$40.00 per property TOTAL FEES ENCLOSED \$1,050.00 Amount to be: refunded charged \$ a. 🔲 A check in the amount of \$ to cover the above fees is enclosed. ь **Ж** Please charge my Deposit Account No. 12-0080 in the amount of \$1,050.00 to cover the above fees. A duplicate copy of this sheet is enclosed. c. 🗷 The Commissioner is hereby authorized to charge any additional fees which may be required, or credit . A duplicate copy of this sheet is enclosed. any overpayment to Deposit Account No. 12-0080 NOTE: Where an appropriate time limit under 37 CFR 1.494 or 1.495 has not been met, a petition to revive (37 CFR 1.137(a) or (b)) must be filed and granted to restore the application to pending status. SEND ALL CORRESPONDENCE TO Elizabeth A. Hanley, Esq. SIGNATURE LAHIVE & COCKFIELD, LLP Elizabeth A. Hanley **NAME** 28 State Street 33,505 Boston, Massachusetts 02109 **United States of America** REGISTRATION NUMBER (617) 227-7400

Form PTO-1390 (REV 10-2000) page 2 of 2

Dated: 27 August 2001

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

#3

In re the application of: Jasper Haeggström et al.

Serial No.: 09/914,451

Priority Date: February 26, 1999

PCT Filing Date: February 28, 2000 (PCT)

U.S. Filing Date: August 27, 2001

For: "Drug Design Based on the Structure of

LTA4 Hydrolase"

Attorney Docket No.: PVZ-006US

Commissioner for Patents BOX SEQUENCE LISTING Washington, D.C. 20231 Group Art Unit: Not Yet Assigned

Examiner: Not Yet Assigned

TRANSMITTAL LETTER FOR DISKETTE CONTAINING SEQUENCE LISTING

Dear Sir:

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Jan

Responsive to the Notification of Missing Requirements Under 35 U.S.C. §371 in the United States Designated/Elected Office (DO/EO/US) dated October 22, 2001, Applicants' attorney submits a diskette containing a computer readable form of the Sequence Listing for the patent application filed on August 27, 2001. The Sequence Listing complies with the requirements of 37 C.F.R. §1.821-1.825. The material on the enclosed diskette is identical in substance to the Sequence Listing appearing on substitute pages 1 and 2 submitted herewith. The computer readable form of the Sequence Listing contained on the enclosed diskette is understood to comply with the requirements of §1.824(d).

"Express Mail" mailing label number_	EL 892 198 215 US
Date of Deposit	December 20, 2001
Postal Service "Express Mail Post Office	ve and is addressed to the Commissioner

Date: December 20, 2001

Respectfully submitted.

LAHIVE & COCKFIELD, LLP

By:

Elizabeth A. Harley Esq Registration No. 33,505 Attorney for Applicants

IN THE UNITED STATES PATENT DESIGNATED OFFICE (DO/US) (National Phase of International App.: PCT/SE00/00384, WO 00/50577)

In re the

application of: Jesper Z. HAEGGSTRÖM et al.

International Application No.: PCT/SE00/00384

International Filing Date: 28 February 2000

U.S. Serial No.: Not Yet Assigned

Filed: Herewith

For: DRUG DESIGN BASED ON THE STRUCTURE OF LTA₄ HYDROLASE

Attorney Docket No.: PVZ-006US

BOX PCT

Commissioner for Patents Washington, D.C. 20231

PRELIMINARY AMENDMENT

Dear Sir:

Preliminary to examination of the above-referenced patent application, please amend the enclosed above-titled International patent application as follows.

In the Claims

Please amend claims 6, 9, 11, 13, 14, 15, 18, 19, 25, 28, 30, and 35 as follows.

- 6. (Amended) A compound which is substantially complementary to a protein according to claim 1.
- 9. (Amended) An isolated complex, which is comprised of a protein according to claim 1 and a complementary compound according to claim 6, wherein the three-

dimensional structure of LTA₄ hydrolase is essentially as disclosed in Table 9 by the parameters defining atom 1- atom 4876, or a functionally equivalent part, derivative or conformational analogue of such a complex.

- 11. (Amended) Use of the parameters of a protein according to claim 1, a compound according to claim 6 in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry.
- 13. (Amended) Use according to claim 11, wherein said drug is for the treatment and/or prevention of disorders involving acute and chronic inflammatory and/or allergic symptoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS).
- 14. (Amended) Use according to claim 11, wherein said drug is for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer.
- 15. (Amended) Use according to claim 11, wherein said drug is for the treatment and/or prevention of disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax.
- 18. (Amended) A method according to claim 16, wherein an enzymatic inhibitor complementary to the amino acids defined in claim 3 is screened for.
- 19. (Amended) An analogue obtainable by the method of claim 16.
- 25. (Amended) A compound obtainable by the method according to claim 21.

- 28. (Amended) A process for the purification of a protein according to claim 1 or obtained according to claim 26, which purification includes hydroxyapatite-based chromatography and a subsequent anion exchange chromatography.
- 30. (Amended) A protein obtained by the method according to claim 26.
- 35. (Amended) A protein according to any one of claims 6, 25, 30 or 31 for use as a medicament.

Please cancel claims 36-38.

REMARKS

Applicant amends the claims to remove multiple dependencies, to provide proper antecedent basis, and to address other matters of form. The foregoing amendments introduce no new matter and are not related to issues of patentability.

Entry of the foregoing Preliminary Amendment is respectfully in order and requested.

Attached hereto as Appendix A is a marked-up version of the changes made to the claims by the current amendments. Appendix A is captioned "Version With Markings To Show Changes Made." Also attached hereto as Appendix B is a complete set of the claims that will be pending upon entry of the amendments presented herein.

If there are any questions regarding the amendments to the application, we invite the Examiner to call Applicant's representative at the telephone number below.

Respectfully submitted,

LAHIVE & COCKFIELD, LLP

Registration No. 33,506 Attorney for Applicants

28 State Street Boston, MA 02109 (617) 227-7400

Date: 27 August 2001

APPENDIX A

VERSION WITH MARKINGS TO SHOW CHANGES MADE

In the Claims

Please amend claims 6, 9, 11, 13, 14, 15, 18, 19, 25, 28, 30, and 35 as follows.

- 6. (Amended) A compound which is substantially complementary to a protein according to any one of claims 1-5.
- 9. (Amended) An isolated complex, which is comprised of a protein according to claims 1-5 and a complementary compound according to any one of claims 6-8, wherein the three-dimensional structure of LTA₄ hydrolase is essentially as disclosed in Table 9 by the parameters defining atom 1- atom 4876, or a functionally equivalent part, derivative or conformational analogue of such a complex.
- 11. (Amended) Use of the parameters of a protein according to any one of claims 1-5, a compound according to any one of claims 6-8 or a complex according to claim 9 or 10 in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry.
- 13. (Amended) Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of disorders involving acute and chronic inflammatory and/or allergic symptoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS).
- 14. (Amended) Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer.

- 15. (Amended) Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax.
- 18. (Amended) A method according to claim 16 or 17, wherein an enzymatic inhibitor complementary to the amino acids defined in any one of claims 3, 4 or 5 is screened for.
- 19. (Amended) An analogue obtainable by the method according to any one of claims 16-18.
- 25. (Amended) A compound obtainable by the method according to any one of claims 21-24.
- 28. (Amended) A process for the purification of a protein according to any one of claims 1-3 or obtained according to claim 26-or 27, which purification includes hydroxyapatite-based chromatography and a subsequent anion exchange chromatography.
- 30. (Amended) A protein obtained by the method according to any one of claims 27-29 26.
- 35. (Amended) A protein according to any one of claims 6-8, 25, 30 or 31 for use as a medicament.

APPENDIX B

- 1. An isolated protein comprising at least a subsequence of the amino acid sequence of LTA₄ hydrolase, which exhibits a three-dimensional form essentially as disclosed in Table 9 by the parameters defining atom 1 to atom 4876, said subsequence being capable of participating in the control of the enzymatic pathway, such as the leukotriene cascade, or a functionally equivalent part, derivative or conformational analogue thereof.
- 2. A protein according to claim 1, which comprises an enzymatically active site defined in the following table:

	Left Wall	Right Wall
1		Lys608, Asp606, Lys605, Lys354, Thr355
2	Phe356, Phe362	Gln544, Asp573, Lys572, Arg568
3	Val376	Lys565, Arg540, Leu507
4	Ser380, Ser352, Glu348	Pro569
5	Tyr378, Glu348	Arg563, Glu533, Phe536, Arg537, Tyr267
6	Tyr383, Phe314, Glu318, Glu384, Arg326	, , , , , , , , , , , , , , , , , , ,
7	Gly268, Gly269, Met270	His295, Asn341, Phe340
8	Ser288, His497	Glu325, Asn291

- 3. A protein according to claim 2, which is an enzyme having a metallohydrolase activity capable of participating in the regulation of enzyme activities in biochemical pathways, wherein said enzymes have structures similar to the ones defined in claim 2.
- 4. A protein according to claim 1, which comprises an enzymatically active site defined by the following amino acids: Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; Glu296; His299; Glu318; Tyr378; Tyr383; Arg563; Lys565.
- 5. A protein according to claim 1, which comprises an enzymatically active site defined by the following amino acids: Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Va1292; His295; Glu296; His299; Trp315; Glu318; Val322; Phe362; Va1367; Leu369; Pro374; Asp375; Ile372; Ala377; Pro382; Tyr378; Tyr383; Arg563; Lys565.

- 6. A compound which is substantially complementary to a protein according to claim 1.
- 7. A compound according to claim 6, which is substantially complementary to an enzymatically active site of said protein and which is capable of specifically inhibiting said enzymatic activity.
- 8. A compound according to claim 7, which is an inhibitor of a metallohydrolase enzyme.
- 9. An isolated complex, which is comprised of a protein according to claim 1 and a complementary compound according to claim 6, wherein the three-dimensional structure of LTA₄ hydrolase is essentially as disclosed in Table 9 by the parameters defining atom 1- atom 4876, or a functionally equivalent part, derivative or conformational analogue of such a complex.
- 10. A complex according to claim 9, wherein the protein complexed with LTA₄ hydrolase is selected from the group which consists of bestatin, thiolamine or hydroxamic acid or a functionally equivalent part, derivative or conformational analogue of such a complex.
- 11. Use of the parameters of a protein according to claim 1, a compound according to claim 6 in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry.
- 12. Use according to claim 11, wherein said parameters are selected from the parameters disclosed in Table 9 defining atom 1- atom 4876.

- 13. Use according to claim 11, wherein said drug is for the treatment and/or prevention of disorders involving acute and chronic inflammatory and/or allergic symptoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS).
- 14. Use according to claim 11, wherein said drug is for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer.
- 15. Use according to claim 11, wherein said drug is for the treatment and/or prevention of disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax.
- 16. A method for screening LTA₄ hydrolase hydrolase analogues that mimic at least a part of 5 the three-dimensional structure of the LTA₄ hydrolase molecule as defined by the parameters shown in Table 9 for atom 1 to atom 4876, which comprises the steps of
- (a) producing a multiplicity of analogue structures of LTA₄ hydrolase and
- (b) selecting an analogue structure, wherein the three-dimensional configuration and spatial arrangement of one or more enzymatically active sites and/or binding sites of said LTA₄ hydrolase remain substantially preserved.
- 17. A method according to claim 16, wherein an analogue exhibiting an enzymatic activity, such as an epoxide hydrolase and/or aminopeptidase activity, is selected.
- 18. A method according to claim 16, wherein an enzymatic inhibitor complementary to the amino acids defined in claim 3 is screened for.
- 19. An analogue obtainable by the method of claim 16.

- 20. An analogue according to claim 19, which exhibits an increased catalytic activity when compared to the naturally occurring form of LTA₄ hydrolase, such as defined in Table 9 by parameters of atom 1 to atom 4876.
- 21. A method for screening LTA₄ hydrolase binding compounds complementary to a region of LTA₄ hydrolase, preferably an enzymatically active site thereof, which comprises the steps of
- (a) producing a multiplicity of possible complementary structures and
- (b) selecting a structure, wherein the three-dimensional configuration and spatial arrangement of regions involved in binding to LTA₄ hydrolase remain substantially preserved, which selection is based on the three-dimensional structure of LTA₄ hydrolase, and/or LTA₄ hydrolase complexed to an inhibitor thereof, in a form adopted thereof in nature, such as defined in Table 9.
- 22. A method according to claim 21, wherein a general metallohydrolase inhibitor is selected, which is capable of inhibiting an enzyme belonging to the M1 family.
- 23. A method according to claim 21, wherein an inhibitor of the epoxide hydrolase activity and/or aminopeptidase activity of LTA₄ hydrolase or of LTA₄ syntheses is selected.
- 24. A method according to claim 21, wherein a compound capable of antagonizing LTB₄ receptor binding of a cell is selected.
- 25. A compound obtainable by the method according to claim 21.
- 26. A method of engineering a protein, which method comprises the steps of
- identification of a suitable set of mutations based on the structure of LTA₄ hydrolase;
- generation of a library of genes which contains the suitable sequence variations;

- selection of clones encoding the LTA₄ hydrolase analogues with a desired activity function;

wherein said desired activity is the capability of efficiently producing an organic compound of interest.

- 27. A method according to claim 26, wherein the specified property is the suicidal mode of action of LTA₄ hydrolase.
- 28. A process for the purification of a protein according to claim 1 or obtained according to claim 26, which purification includes hydroxyapatite-based chromatography and a subsequent anion exchange chromatography.
- 29. A process for the crystallization of an LTA₄ hydrolase, an analogue or a derivative thereof, wherein said crystallisation is performed with the addition of an ytterbium salt as an additive, such as an ytterbium chloride.
- 30. A protein obtained by the method according to claim 26.
- 31. A protein according to claim 30, which is present in an essentially pure form.
- 32. An isolated nucleic acid encoding a protein according to claim 30 or 31.
- 33. A nucleic acid capable of specifically hybridising to a nucleic acid according to claim 32.
- 34. Use of a protein, which is a genetically modified LTA₄ hydrolase, according to claim 30 or 31 in the preparation of LTB₄ or other metabolites in the leukotriene cascade.
- 35. A protein according to any one of claims 6, 25, 30 or 31 for use as a medicament.

JC03 Rec'd PCT/PTO 2 7 AUG 2001

WO 00/50577

PCT/SE00/00384

DRUG DESIGN BASED ON THE STRUCTURE OF LTA4 HYDROLASE

1. BACKGROUND

1.1 Technical field

The present invention relates to methods of design or identification of biologically active compounds, which methods are based on the first definition ever of a three-dimensional structure of a protein involved in the leukotriene cascade. Further, the invention relates to novel compounds obtained by said methods, to advantageous uses of such compounds as well as to processes for the preparation thereof.

1.2 Prior art

Leukotriene A4 (LTA₄) hydrolase is a pivotal enzyme in the biosynthesis of leukotrienes, a family of paracrine hormones implicated in the pathophysiology of inflammatory and allergic disorders, in particular bronchial asthma (Samuelsson, B. Science 220, 568-75 (1983); and Lewis, R.A., Austen, K.F. & Soberman, R.J. N Engl J Med 323, 645-55 (1990)). Leukotrienes are formed by immunocompetent cells including neutrophils, eosinophils, basophils, mast cells, and macrophages, in response to a variety of immunological as well as non-immunological stimuli. These lipid mediators are divided into two major classes exemplified by the chemotaxin LTB4, and the spasmogenic cysteinyl-leukotrienes (LTC4, LTD4, and LTE4). Leukotriene biosynthesis is initiated by the enzyme 5-lipoxygenase which converts arachidonic acid into the unstable epoxide LTA4, a central intermediate in the leukotriene cascade. LTA4 may in turn be hydrolyzed into LTB4 by the enzyme LTA4 hydrolase, or conjugated with GSH to form LTC4, a reaction catalyzed by a specific LTC4 synthase. During cellular activation, all key enzymes in leukotriene biosynthesis, except LTA4 hydrolase, form a biosynthetic complex assembled at the nuclear membrane, suggesting that leukotrienes may have unknown intranuclear functions related to gene regulation or cell growth (Serhan, C.N., Haeggstrom, J.Z. & Leslie, C.C. Faseb J 10, 1147-58 (1996)).

Leukotriene B4, the natural product of LTA4 hydrolase, is one of the most powerful chemotactic agents known to date and triggers leukocyte adherence and ag-

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gregation at only nM concentrations (Ford-Hutchinson, A.W., Bray, M.A., Doig, M.V., Shipley, M.E. & Smith, M.J.H. Nature 286, 264-265 (1980)). Hence, this molecule is regarded as a key mediator of inflammation, and has been implicated in a number of diseases, including arthritis, psoriasis, inflammatory bowel disease (IBD), and chronic obstructive pulmonary disease (COPD). Furthermore, the role of LTB4 in inflammation has been well corroborated by the anti-inflammatory properties of LTA4 hydrolase inhibitors, particularly in combination with a cyclooxygenase inhibitor, and specific LTB4 receptor antagonists, as well as the reduced inflammatory reactions observed in several animal models of leukotriene deficiency (Tsuji, F., Miyake, Y., Enomoto, H., Horiuchi, M., Mita, S. Eur. J. Pharmacol. 346, 81-85, (1998); Chen, X.S., Sheller, J.R., Johnson, E.N. & Funk, C.D. Nature 372, 179-182 (1994); Griffiths, R.J., et al. Proc Natl Acad Sci USA 92, 517-21 (1995); and Griffiths, R.J., et al. J Exp Med 185, 1123-9 (1997)). In addition, LTB4 modulates the immune response, e.g., by interference with specific subsets of lymphocytes, production of cytokines, as well as liberation of immunoglobulins from B-lymphocytes (Payan, D.G., Missirian-Bastian, A. & Goetzl, E.J. Proc Natl Acad Sci U S A 81. 3501-5 (1984); Rola-Pleszczynski, M. & Lemaire, I. J Immunol 135, 3958-61 (1985); and Yamaoka, K.A., Claesson, H.E. & Rosen, A. J. Immunol 143, 1996-2000 (1989)). Recent data also indicate that LTB4 stimulates, and thus has a crucial role in the regulation of, cell proliferation and cell survival in HL-60 cells, suggesting that LTA4 hydrolase inhibitors may have an anti-proliferative effect. (Dittman, K.H., Mayer, C., Rodemann, H.P., Petrides, P.E., and Denzlinger, C. Leuk, Res. 22. 49-53 (1998)). The cell surface receptor for LTB4 (BLTR) was recently cloned and found to be abundantly expressed in the immune system, including lymphocytes, spleen and thymus (Yokomizo, T., Izumi, T., Chang, K., Takuwa, Y. & Shimuzu, T. Nature 387, 620-624 (1997)). BLTR belongs to a family of chemokine receptors and, interestingly, together with CD4 it was found to be an efficient coreceptor for HIV-1 infection (Owman, C., et al. Proc Natl Acad Sci USA 95, 9530-4 (1998)). Moreover, LTB4 is also a natural ligand to the nuclear orphan receptor PPARa.

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suggesting that LTB4 may have intranuclear functions possibly related to lipid homeostasis (Devchand, P.R., et al. Nature 384, 39-43 (1996)).

LTA4 hydrolase is a cytosolic 69 kDa enzyme without any similarity to other soluble or membrane bound xenobiotic epoxide hydrolases (Funk, C.D., et al. Proc Natl Acad Sci U S A 84, 6677-81 (1987)). The enzyme's epoxide hydrolase activity, which generates LTB4, is highly substrate selective accepting only LTA4 and to a small extent the double bond isomers LTA3 and LTA5. Typically, LTA4 hydrolase undergoes suicide inactivation and covalent modification when exposed to LTA4 (Evans, J.F., Nathaniel, D.J., Zamboni, R.J. & Ford-Hutchinson, A.W. J. Biol. Chem. 260, 10966-10970 (1985)). During this process, LTA4 apparently binds to Tyr-378, a residue which also seems to play a role for the formation of the critical cis-trans-trans geometry in the conjugated triene structure of LTB4 (Mueller, M.J., et al. Proc Natl Acad Sci U S A 93, 5931-5935 (1996); and Mueller, M., Andberg, M., Samuelsson, B. & Haeggstrom, J. Z. J. Biol. Chem. 271, 24345-24348 (1996)).

From sequence comparisons with certain metalloproteases and aminopeptidases, a zinc binding motif (HEXXH-X18-E) was unexpectedly found in LTA4 hydrolase (Vallee, B.L. & Auld, D.S. Proc. Natl. Acad. Sci. USA 87, 220-224 (1990)). Further studies demonstrated that the enzyme indeed contains one catalytic zinc atom complexed to His295, His299, and Glu318 (Medina, J.F., et al. Proc. Natl. Acad. Sci. USA 88, 7620-7624 (1991)). In addition, a previously unknown peptide cleaving activity was discovered which requires the presence of anions, particularly chloride (Haeggström, J.Z., Wetterholm, A., Medina, J.F. & Samuelsson, B. J Lipid Mediator 6, 1-13 (1993)). Although the endogenous physiological peptidase substrate(s) has not yet been identified, LTA4 hydrolase cleaves certain arginyl di- and tripeptides with very high efficiency (Örning, L., Gierse, J.K. & Fitzpatrick, F.A. J. Biol. Chem. 269, 11269-11273 (1994)). Hence, LTA4 hydrolase can be described as a bifunctional zinc metalloenzyme with the unique ability to accept both lipid and peptide substrates. Using site-directed mutagenesis, Glu296 and Tyr383 were found to be critical for the peptidase reaction, presumably as a general base and proton donor, respectively (Blomster, M., Wetterholm, A., Mueller, M.J. & Haegeström

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J.Z. Eur. J. Biochem. 231, 528-534 (1995); and Wetterholm, A., et al. Proc Natl Acad Sci U SA 89, 9141-9145 (1992)). Since the enzyme's ability to convert LTA4 into LTB4 was not affected by the mutations, the two enzyme activities of LTA4 hydrolase are exerted via non-identical but overlapping active sites. Notably, unlike other enzymes in the leukotriene cascade, LTA4 hydrolase is ubiquitous in mammalian cells and tissues suggesting that it may have other functions presumably related to its peptide cleaving activity.

As a consequence of the identification of LTA₄ hydrolase as a zinc metalloen-zyme with a peptidase activity, it was observed that LTA₄ hydrolase is inhibited by bestatin, a general aminopeptidase inhibitor, and captopril, an inhibitor of angiotensin converting enzyme (Örning, L., et al. J. Biol. Chem. 266, 16507-16511 (1991)).

Tsuge et al., (J. Mol. Biol. 238,854-856 (1994)), have described the crystallization of LTA₄ hydrolase. However, despite the well recognized need thereof, the three-dimensional structure of LTA4 hydrolase has not yet been disclosed. More specifically, the problems that need to be overcome in order to provide such a determination may in brief be explained as follows. There are two major difficulties in obtaining a three-dimensional structure of a protein molecule. The first one is to grow crystals of good quality that are reproducible and diffract to atomic resolution (beyond 2.5Å). This means a thorough and cumbersome investigation of parameters that influence the crystal growth such as pH, temperature, nature of buffers, nature of precipitant, just to mention a few. The addition of ligands such as substrate analogues or inhibitors or the addition of other molecules can be important for obtaining good crystals. There is only little understanding of the physical background of the crystallisation process which means that the search for suitable crystallisation conditions for a certain protein is unique, requires creativity and intuition, and is governed by trial and error procedures. The purity of the protein is also a crucial parameter in the crystallisation and a suitable degree of purity can be hard, or even imposible, to achieve. The second major difficulty is associated with overcoming the phase-problem which is inherent to X-ray diffraction methods. To be able to overcome this problem it is necessary to substitute the protein with suitable heavy

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atom substance such as e.g. mercury, gold or platinum compounds. Crystals often cannot withstand the treatment with these compounds and the search for suitable substitutions is not straight forward and may become very exhaustive. Another option is to substitute all methionines by seleno-methionine (Se-Met) residues. This method requires production of recombinant protein in special strains of E. coli under non-standard conditions, followed by a new purification and recrystallisation of the Se-Met containing protein. Although Tsuge et al reported the crystallisation of LTA4 hydrolase, their crystals only diffracted to medium resolution and the phaseproblem was not solved. Thus, as a reliable definition of the three-dimensional structure of LTA₄ hydrolase would enable e.g. a display in visual form on a computer screen of the shape of the molecule, then, could the above mentioned problems be solved, a whole range of possibilities would be opened, such as rational structure-based drug design, e.g. in combination with combinatorial chemistry, aimed at production of novel medicaments useful in disorders associated with the leukotriene cascade, as well as protein-engineering to create novel variants of the enzyme with altered, but yet useful, catalytic properties.

As LTA4 hydrolase is a recognized important drug target, some inhibitors thereof have been synthesized (Wetterholm, A., et al. J Pharmacol Exp Ther 275, 31-7 (1995); and Yuan, W., Wong, C., Haeggstrom, J. Z., Wetterholm, A. & Samuelsson, B. J. Am. Chem. Soc., 114, 6552-6553 (1992)). Interestingly, certain inhibitors of LTA4 hydrolase were reported to act also as LTB4 receptor antagonists (Labaudinière R, Hilboll G, Leon-Lomeli A, Terlain B, Cavy F, Parnham M, Kuhl P, and Dereu N. J. Med. Chem. 35, 3170-3179 (1992)). Due to the absence of any available information regarding the three-dimensional structure of LTA4 hydrolase, as discussed above, none of the previously described inhibitors have been designed based on the exact structure thereof. Accordingly, there is a need within this field of determining the three-dimensional structure of LTA4 hydrolase in order to design more potent and selective inhibitors of LTA4 hydrolase as well as modified structures exhibiting even more advantageous pharmaceutical properties.

2. THE PRESENT INVENTION

As the following chapter includes a substantial amount of text, it has herein been divided into separate sections, each one of which disclose separate aspects of the present invention.

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2.1 Summary of the invention

The object of the present invention is to fulfill the above defined need. This has been achieved by the crystallization and determination of the three-dimensional structure of LTA4 hydrolase complexed with the competitive inhibitor bestatin and subsequent structure determination of complexes between LTA4 hydrolase and two specific inhibitors. It is the first three-dimensional structure of any protein component of the leukotriene cascade and enables a description of the structural basis and molecular mechanisms of various enzyme functions, such as the two catalytic activities of LTA4 hydrolase. In addition, the structural information will now make possible rational design of enzyme inhibitors, which may be developed into clinically useful anti-inflammatory drugs.

2.2 Brief description of the drawings

Figure 1 shows the key enzymes and intermediates in leukotriene biosynthesis.

Figure 2 shows 2Fo-Fc density contoured at 1.1 s. Part of the active site in the neighborhood of the bestatin molecules is shown.

Figure 3 is a ribbon diagram of the tertiary structure of leukotriene A4 hydrolase.

Figure 4 shows ribbon diagrams of the N-terminal domains of . LTA₄ hydrolase.

Figure 5 shows ribbon diagrams of the catalytic domain of LTA₄ hydrolase and therolysin.

Figure 6 shows the structure of the C-terminal domain.

Figure 7 illustrates zinc binding ligands in LTA4 hydrolase.

Figure 8 (a) is a Ball-and-Stick presentation of the binding of bestatin in LTA4 hydrolase, while Figure 8 (b) is a schematic overview of bestatin binding in LTA4 hydrolase.

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Figure 9 (a) is a wire representation of the central cavity found in LTA4 hydrolase (shown as $C\alpha$ -trace).

Figure 9 (b) is a schematic presentation for the proposed binding of LTA4 into the cavity.

Figure 10 is a schematic representation for the proposed reaction mechanism of the epoxide hydrolase.

2.3 Definitions

In the present context, the term "the three-dimensional form adopted thereof in nature" is to be understood as the conformational structure, defined by the parameters x, y and z in a conventional coordinate system, that a naturally occurring molecule adapt under conditions where it is capable of exerting its biological activities.

The specific conditions during which the herein presented data were collected are detailed in the section "Experimental".

The term "isolated" and variations thereof when used in connection with a molecule, such as protein, a polypeptide or a nucleic acid, means that said molecule is isolated from other substances, such as other proteins, DNA etc normally accompanying it in its natural environment.

The term "leukotriene A₄ (LTA₄) hydrolase" as used herein is to be understood to include any mammalian or other LTA4 hydrolase which comprises the same backbone as the human form specifically disclosed in the present application, irrespective of source. The amino acid sequences of mammalian LTA₄ hydrolase have been shown to be identical to about 90%. Thus, the three-dimensional structures thereof may be suspected to be identical to approximately the same extent.

"Thiolamine" and "hydroxamic acid" are used herein to denote the compounds examplified in the Experimental section of the present specification.

A "complementary compound" means any compound, the structure of which enables a binding thereof to a specified protein, i.e a compound having a conformation or structure enabling such a suitable fit as to provide an energetically favorable interaction between protein-complementary compound.

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"Analogue" means, as used herein, a chemically altered molecule which shares the backbone with, or at least structurally resembles, a "parent molecule". In the present specification, such a "parent molecule" may be LTA₄ hydrolase or an inhibitor thereof.

In the present application, the term "active site" is to be understood to include any region capable of binding a substrate and converting it into product.

The term "nucleic acid" refers to a deoxyribonucleotide or ribonucleotide polymer in either single- or double-stranded form, and unless otherwise limited, encompasses known analogs of nucleotides, that can function in a similar manner as naturally occurring nucleotides.

The phrase "hybridising specifically to" refers to the binding, duplexing, or hybridising of a molecule only to a particular nucleotide sequence under stringent conditions when that sequence is present in a complex mixture (e.g., total cellular) of DNA or RNA. The term "stringent conditions" refers to conditions under which a probe will hybridise to its target subsequence, but to no other sequences. Stringent conditions are sequence-dependent and will be different in different circumstances. Longer sequences hybridise specifically at higher temperatures. Generally, stringent conditions are selected to be about 5°C lower than the thermal melting point Tm for the specific sequence at a defined ionic strength and pH. The Tm is the temperature (under defined ionic strength, pH, and nucleic acid concentration) at which 50% of the probes complementary to the target sequence hybridise to the target sequence at equilibrium. (As the target sequences are generally present in excess, at Tm, 50% of the probes are occupies at equilibrium). Typically, stringent conditions will be those in which the salt concentration is less than about 1.0 M Na ion, typically about 0.01 to 1.0 M Na ion concentration (or other salts) at pH 7.0 to 8.3 and the temperature is at least about 30°C for short probes (e.g., 10 to 50 nucleotides) and at least about 60°C for long probes (e.g., greater than 50 nucleotides). Stringent conditions may also be achieved with the addition of destabilizing agents such as formamide.

"Essentially pure" means herein a purity of at least about 80%, especially at least about 90% and preferably at least about 95%, such as 98-99%. The purity of

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LTA₄ hydrolase, an analogue or inhibitor thereof is according to the present invention preferably determined by general biochemical and biophysical methods well-known to the skilled in this field. For proteins, SDS polyacrylamide gel electrophoresis (SDS-PAGE) with Coomassie and silver staining or amino acid sequence analysis can be used, whereas high-pressure liquid chromatography (HPLC), gas chromatography coupled to mass spectrometry (GC-MS), and nuclear magnetic resonance spectroscopy (NMR) are suitable methods for small organic molecules (peptides, lipids, or carbohydrates, or combinations of these classes of substances).

2.4 Detailed description of the invention

2.4.1 LTA₄ hydrolase, subsequences and analogues thereof

In a first aspect, the present invention relates to an isolated protein comprising at least a subsequence of the amino acid sequence of leukotriene A₄ (LTA₄) hydrolase, which subsequence has the corresponding three-dimensional form adopted thereof in nature. The protein according to invention as discussed below and elsewhere in this application is also understood to encompass any other functionally equivalent part, derivative or conformational analogue thereof. More specifically, the invention relates to the above disclosed protein which comprises a subsequence of the amino acid sequence of leukotriene A₄ (LTA₄) hydrolase, which is able to participate in, and influence, e.g. by providing enzymatic activity, the leukotriene cascade. Most preferably, the protein according to the invention is capable of controling said cascade by exerting an enzymatic activity and thus regulate the production of leukotriene B₄ (LTB₄). In a particular embodiment, the protein is comprised of essentially all of the amino acid sequence of leukotriene A₄ (LTA₄) hydrolase as disclosed in SEQ ID NO 1, or a functionally equivalent part, derivative or conformational analogue thereof.

Thus, the present invention relates to an isolated LTA₄ hydrolase in its naturally occurring three-dimensional form. More specifically, the present application provides a listing illustrating, for the first time, the coordinates defining human LTA₄ hydrolase complexed to an inhibitor thereof. Thus, the coordinates defining the conformation of LTA₄ hydrolase have been determined by the present inventors as com-

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plexed with bestatin, thiolamine and hydroxamic acid, respectively. Bestatin is a universal inhibitor of amino peptidase activity (see e.g. Mathé, G. Biochem. Pharmacol. 45, 49-54 (1991)), while the last mentioned two are specific inhibitors of LTA₄ hydrolase. Based on these different activities, said inhibitors may be used as models in the design of novel molecules having desired properties. Methods for such design will be discussed in further detail below as a further advantageous aspect of the invention. For reasons of convenience for the reader of the present specification, the data collection comprising the novel coordinates according to the invention is included in the present description as a separate section denoted "X-ray data", as Table 9, immediately preceding the claims. In said table, atom no 1 to atom no 4876 define the LTA₄ hydrolase part of the complex. (protein part), atom no 4877 refers to Zn, atom nos. 4878-4880 refer to Yb, atom nos. 4881-4885 refer to imidazole, atom nos. 4886-4889 refer to acetate, atom nos 4890-4908 refer to thiolamine while atom nos. 4909-5160 refer to water. Thus, the intervening atoms relate to the metals that bind in LTA₄ hydrolase, i.e. the active site Zn atom and the Yb atoms that were crucial for the present structure determination. The conditions prevailing at the determination thereof will be described in detail in the Experimental section below. As the skilled in this field realises, such coordinates usually exhibit a certain degree of variation, due to e.g. thermal motion and slight differences in crystal packing. Thus, any references herein to Table 9 in connection with the proteins and other molecules are merely intended to illustrate an average value for each of the coordinates defining the conformation of the molecules under identical conditions, as determined by use of the same apparatus and method. Accordingly, this embodiment of the invention is not limited to a molecule having exactly the specified coordinates, but rather to molecules capable of adopting such a structure. For example, a human LTA₄ hydrolase according to the invention will exhibit a strong bit a conformational similarity with the coordinates presented by atom nos 1 -4876 of Table 9, wherein a variation of about 1%, or 0.5 Å, may be expected. Accordingly, any such variants are within the scope of the present invention.

As regards amino acid sequence, in a specific embodiment, the protein according to the invention is identical, by direct sequence comparison, to at least about

50%, more specifically, at least about 70%, such as at least about 90%, to the LTA₄ hydrolase as defined by SEQ ID NO. 1 while in the three-dimensional form adopted thereof in nature. In this context, it is noted that the amino acid sequence of LTA₄ hydrolase also appears from the data of Table 9, but is also included as a separate sequence listing for reasons of clarity. The protein of this embodiment of the invention are e.g. variants originating from any species, preferably mammals, such as humans, mice or other rodents, etc. Alternatively, the variants including subsequences of the human sequence are mutated forms, resulting from either spontaneous mutations or deliberately produced mutations, as discussed in more detail below.

One preferred embodiment of the present invention is a protein which comprises at least one of the regions defined below in Tables 1-3 below as active sites.

Table 1: Residues lining the big cavity from outsite to insite

	Left wall	Right wall
1		Lys608, Asp606, Lys605,
		Lys354, Thr355
2	Phe356, Phe362	Gln544, Asp573, Lys572, Arg568
3	Val376	Lys565, Arg540, Leu507
4	Ser380, Ser352, Glu348	Pro569
5	Tyr378, Glu348	Arg563, Glu533, Phe536,
•		Arg537, Tyr267
6	Tyr383, Phe314, Glu318, Glu384,	
	Arg326	
7	Gly268, Gly269, Met270	His295, Asn341, Phe340
8	Ser288, His497	Glu325, Asn291

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In Table 1, Lys565, Ser380, Pro569, Glu533, Tyr383, Phe314, Glu318, Glu384, Arg326, Gly268, Gly269, Met270, His295, Phe340, Ser288, and Glu325 are strictly conserved amino acids, while Lys608, Phe356, Phe362, Lys572, Arg568, Tyr378, Phe536, Tyr 267, and Asn291 are conserved in nature.

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Table 2: Amino-acids in the bestatin binding site ("basic" amino-peptidase site)
The binding of bestatin to LTA₄ hydrolase may also be described by way of coordinates. Below follows the specific amino acids involved in the binding of bestatin and similar structures, as defined according to the invention.

Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; Glu296; His299; Glu318; Tyr378; Tyr383; Arg563; Lys565.

Table 3: Amino acids in the leukotriene binding site

The present amino acids define the site binding leukotriene-based inhibitors, such as thiolamine and hydroxamic acid, as shown in Table 9 for thiolamine.

Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; Glu296; His299; Trp315; Glu318; Val322; Phe362; Val367; Leu369; Pro374; Asp375; Ile372; Ala377; Pro382; Tyr378; Tyr383; Arg563; Lys565.

In Tables 1-3 above, the enumeration of the amino acid sequence of LTA₄ hydrolase begin without the initial Met. Thus, compared to SEQ ID NO 1, which includes the initial Met, the amino acid enumeration above is lowered by one. Accordingly, Gln136 above corresponds to Gln 137 of SED ID NO 1, Ala137 above corresponds to Ala 138 of SEQ ID NO 1, etc.

Table 4: General catalytic domain for the M1 class of enzymes Amino acids no. 210-450.

The present region will provide a basis for the development of enzyme inhibitors useful in the control other biological pathways than the leukotriene cascade.

Thus, as regards the above defined region of aminopeptidase activity of LTA₄ hydrolase, the present inventors have surprisingly observed, that said region is in fact universal for all enzymes belonging to the metallohydrolase family denoted M1.

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Thus, this specific subsequence of LTA₄ hydrolase is encompassed by the present invention as a novel protein *per se*. In addition to the various advantageous uses of subsequences of LTA₄ hydrolase described herein in connection with the leukotriene cascade, this region, which is shared between all M1 enzymes, will find several further applications in connection with other enzymatic pathways. For example, the present region, herein denoted the "M1 region" in order to clarify that it is shared between the M1 enzymes, may advantageously be used to produce synthetic inhibitors, or identify natural inhibitors, of any one of the other M1 enzymes. Such M1 inhibitors will be discussed below when compounds complementary to LTA₄ hydrolase are disclosed.

The above disclosed proteins and peptides comprising subunits of LTA₄ hydrolase are advantageously used e.g. as enzymes or more preferably in methods wherein novel inhibitors of enzymatic activities are identified and/or designed.

2.4.2 Compounds complementary to LTA₄ hydrolase

In a second aspect, the present invention relates to a novel compound defined by a structure substantially complementary to the above described protein, preferably identified by use of the novel LTA₄ hydrolase conformation according to the present invention. The complementary compound is a naturally occurring or synthetic protein, peptide, lipid, carbohydrate or any other organic or inorganic compound. In relation to naturally occurring compounds, it is to be understood that the present invention relates to such compounds as isolated from their natural environment, preferably identifiable by aid of the novel coordinates defining structures according to the invention, as examplified by the complementary compounds used in the complexes shown in Table 9.

In a first embodiment, the present complementary compound is substantially complementary to an enzymatically active site of the protein and is advantageously capable of specifically inhibiting an enzymatic activity of said protein. Thus, in one embodiment, the present compound is substantially complementary to parts, or all, of the "basic" aminopeptidase binding site defined in Table 2 above. Thus, the pres-

ent compound is an inhibitor capable of specifically inhibiting an aminopeptidase activity of an enzyme, preferably of LTA₄ hydrolase. In an alternative embodiment, the present compound is substantially complementary to parts, or all, of the leukotriene binding site as defined in Table 3 above. Thus, the present compound is an inhibitor capable of specifically inhibiting an epoxide hydrolase activity of an enzyme, preferably of LTA₄ hydrolase. (The inhibition of both aminopeptidase and epoxidase hydrolase is discussed in detail below in the experimental section.) As the present two binding sites of LTA₄ hydrolase overlap in part, a further embodiment is a compound which is complementary to essential parts of both of the above discussed two binding sites, in part or partially, which thus preferably is an inhibitor of both the discussed activities.

As already mentioned above, one compound which is complementary to an enzymatically active site of LTA₄ hydrolase is a compound complementary to the M1 region thereof and thus capable of partial or total inhibition of the enzymatic activity of LTA₄ hydrolase or any other metallohydrolase belonging to the M1 family. In the present application, such inhibitors will be denoted M1 inhibitors.

As the skilled in this field will realise, the present inhibitors disclosed above need not be compound that inhibit a biological activity completely, but may be capable of exerting a partially inhibiting activity, i.e, lowering the enzymatic activity.

In another embodiment, the present complementary compound is a compound which is also capable of binding to the receptor for the product of an LTA₄ hydrolase, i.e. an LTB₄ receptor, e.g. on a cell, such as a polymorphonuclear leukocyte. Thus, such a compound may be useful as an LTB₄ antagonist whereby the biological effect of LTA₄ hydrolase activity may be regulated. Accordingly, any such LTB₄ antagonist designed and/or identified using the coordinates of LTA₄ hydrolase as presented herein are also encompassed by the present invention.

In another embodiment, the present complementary compound is a compound which, apart from being capable of binding to an active site of LTA4 hydrolase, is also capable of binding to an active site of LTC4 synthase which binds the same substrate as LTA4 hydrolase, i.e. LTA4, and turns it over into LTC4 (cf. Fig 1) and

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is thus expected to share important structural features with the active site of LTA4 hydrolase. Such a compound may be useful as an inhibitor of LTC4 biosynthesis, whereby the production thereof may be regulated. Accordingly, any such LTC4 synthase inhibitor, designed and/or identified using the coordinates of LTA4 hydrolase, are also encompassed by the present invention.

The specific properties and advantageous uses of the present compounds as well as the design and production of novel LTA₄ hydrolase inhibitors will be described in further detail below in relation to the various methods.

2.4.3 A complex of LTA₄ hydrolase and a complementary compound

In a third aspect, the present invention relates to an isolated complex comprised of a protein as described above and a compound complementary to said protein. Said complementary compound may thus be an inhibitor of one or more of the protein's enzymatic activities, such as an aminopeptidase and/or epoxide hydrolase activity, such as bestatin, hydroxamic acid or thiolamine, or leukotriene B4 or any analogue thereof, or LTC₄ or any analogue thereof. Examples of complementary compounds are bestatin, thiolamine or hydroxamic acid. In the present context, it is to be understood that the invention also relates to specific regions of said inhibitors. that have never been specifically disclosed for the present purpose, as well as novel inhibitors identified by aid of the present invention. In specific embodiments, the complex according to the invention is composed of LTA₄ hydrolase complexed with bestatin, thiolamine or hydroxamic acid, respectively, wherein the LTA₄ hydrolase is as defined by the coordinates presented in Table 9, or any functional fragment, derivative or analogue thereof. As bestatin is aminopeptidase based, further similar and advantageous inhibitors may be developped based on the structural information for LTA₄ hydrolase complexed with bestatin, preferably combined with the specification of the binding site of Table 2. Further, as both thiolamine is leukotriene based, the information provided in Table 9, preferably combined with the specification of binding site of Table 3, will prove to be an advantageous tool in order to gain more information about such enzymatic binding and thus the development of further

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novel inhibitors, the same principles applying to hydroxamic acid, which is also leukotriene based.

Accordingly, the present invention presents for the first time the coordinates defining the three-dimensional structure of a complex of LTA₄ hydrolase and an inhibitor thereof as determined by X-ray crystallography, e.g. as illustrated in Table 9. In fact, this is the first time ever to disclose the exact parameters defining the three-dimensional structure of a protein component of the leukotriene cascade. Due to these novel reliable parameters, the complex as well as the components thereof are readily distinguished from the prior art. Together with biochemical and mutagenetic data, the novel structures will provide the basis for understanding the molecular mechanisms of the aminopeptidase and epoxide hydrolase activities, as well as the enzyme's suicide inhibition. Accordingly, the present invention will open a whole range of new possibilities as regards e.g. identification and/or design of novel biologically active molecules and methods of controlling said cascade, *in vivo* or *in vitro*. Consequently, novel advantageous drugs, such as medicaments for the treatment and/or prevention of inflammatory and/or allergic diseases, may be designed, as will be discussed in further detail below.

In the present context, it is to be understood that proteins according to the invention include the naturally ocurring three dimensional forms thereof, separated and isolated from its natural environments, as well as any such protein, wherein deletions, additions and/or substitutions of the amino acid sequence have been made, provided that the three dimensional structure is substantially maintained, as the exerted biological activity is critically dependent upon the particular three-dimensional folding of the protein. The present invention also encompasses any derivative or conformational analogue of the above disclosed proteins, which has a three-dimensional structure essentially as disclosed above, or an effective part thereof having the biological activities discussed in detail below.

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2.4.4 Advantageous uses of LTA₄ hydrolase, complementary compounds and complexes thereof

A fourth aspect of the present invention is the use of a protein, a complementary compound or a complex according to to the invention in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry. Such methods will be disclosed in detail below. The drugs designed using the above mentioned compounds may be suitable for the treatment and/or prevention of disorders involving acute and chronic inflammatory symtoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS). Further, such a drug may be useed for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer. Alternatively, a drug may be designed which is effective for the treatment and/or prevention of an inflammatory and/or allergic disorders caused by the lethal factor of Bacillus anthracis, e.g. anthrax. However, the above mentioned diseases are exemplary and other diseases or conditions not mentioned herein may also be contemplated.

In a further aspect, the present invention relates to the use of a protein having a structure substantially as defined for the LTA₄ hydrolase of the invention, or a part, analogue or derivative thereof, for screening a compound for possible medicinal activity. In the pharmaceutical industry, new or known compounds are routinely screened for new uses employing a variety of known *in vitro* or *in vivo* screens. Often such screens involve complex natural substances and are consequently expensive to carry out, and the results may be difficult to interpret. However, the knowledge of the three-dimensional protein structure according to the invention allows a preliminary screening to be carried out on the basis of the three-dimensional structure of a region thereof, and the structural similarity of a molecule which is being screened. Such screening can conveniently be carried out using computer modelling techniques, which match the three-dimensional structure of the protein or part thereof with the structure of the molecule being screened. Potential agonist or inhibitor activity may be predicted. As a result, the production efficiency, bioavail-

ability, immunogenicity, stability etc. may be favourably changed with respect to their therapeutic application.

As regards the above disclosed M1 inhibitors, these compounds will presumably find a broader field of application than the other novel inhibitors according to the invention. Thus, the novel general M1 inhibitors are advantageously used e.g. in models to disclose in further detail other enzymatic pathways. Further, they may also be used in the above mentioned type of methods of drug design etc.

2.4.5 Screening for LTA₄ hydrolase analogues

2.4.5 (a) Method

Accordingly, in another aspect, the invention relates to a method for screening LTA₄ hydrolase analogues that mimic at least a part of the three dimensional structure of LTA₄ hydrolase, which comprises the steps of

- (a) producing a multiplicity of analogue structures of the LTA₄ hydrolase
- (b) selecting an analogue structure represented by a three-dimensional representation wherein the three-dimensional configuration and spatial arrangement of specific regions, preferably involved in ligand binding of said LTA₄ hydrolase, remain substantially preserved.

The coordinates used are general for LTA₄ hydrolase are essentially as illustrated in Table 9, as defined by atom nos. 1-4876.

More specifically, analogue structures of LTA4 hydrolase may be screened by their ability to catalyze a particular reaction which may be monitored by chemical physical or immunological means. Furthermore, the analogue structure may be selected from its ability to produce receptor ligands or inhibitors of secondary reactions, which may be monitored directly, as examplified above, via binding assays, enzyme assays, chemical assays, or functional bioassays.

Thus, in one embodiment, the invention relates to a method of screening, wherein one or more analogues exhibiting epoxide hydrolase activity, are screened for. Thus, such a method may be based on the data of Table 9, wherein the binding of thiolamine to LTA₄ hydrolase is shown, preferably combined with the information of Table 3 regarding the active site of LTA₄ hydrolase. In one embodiment, the

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invention relates to a method of screening, wherein one or more analogues exhibiting epoxide hydrolase activity, are screened for. In an alternative embodiment, the present method is used to screen for analogues exhibiting aminopeptidase activity, which method e.g. is based data concerning the binding of bestatin to LTA₄ hydrolase is used, preferably combined with the information of Table 2 regarding the active site of LTA₄ hydrolase. Thus, the present analogues will comprise a region which is essentially analogue with the regions of LTA₄ hydrolase exhibiting aminopeptidase activity, and/or analogues exhibiting epoxide hydrolase activity are selected.

In an advantageous embodiment of the screening method according to the invention, one or more analogues comprising one or more genetic modifications, as compared to the naturally occurring form of LTA₄ hydrolase, are selected.

2.4.5 (b) Analogues obtainable by the present screening method

Further, the invention also relates to a novel analogue obtainable by the method according to the invention, such as an analogue exhibiting an increased or improved or otherwise modified catalytic activity when compared to the naturally occurring form of LTA₄ hydrolase. Preferably, said catalytic activity is an epoxide hydrolase and/or aminopeptidase activity. Further, the invention relates to an analogue obtainable by the present method and capable of acting as a metallohydrolase, preferably belonging to the M1 class of metallohydrolases.

2.4.5 (c) Mutated forms of LTA₄ hydrolase obtainable by the present screening method

In one advantageous embodiment, the present invention relates to a specified analogue which is a mutated form of LTA₄ hydrolase, which analogue comprises one or more of the mutations defined in the following Tables 5-7, wherein amino acids are given in single letter code. Thus,

Q134G/A/V/L/I/S/T/D/E/N/R/H/K/P/C/M/F/Y/W indicates that residue glutamine 134, using the LTA4 hydrolase numbering scheme, is modified to an alanine, valine, a leucine and so forth.

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Table 5: Mutations in the active site

	Q134G/A/V/L/I/S/T/D/E/N/R/H/K/P/C/M/F/Y/W	5(1)
	Q136G/A/V/L/I/S/T/D/E/N/R/H/K/P/C/M/F/Y/W	5(2)
5	A137G/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(3)
	Y267G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W	5(4)
	G268A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(5)
	G269A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	56)
*	M270G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/F/Y/W	5(7)
10	E271G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	5(8)
	V292G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(9)
	H295/G/A/V/L/I/S/T/D/E/N/Q/R/K/P/C/M/F/Y/W	5(10)
	E296/G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	5(11)
	H299G/A/V/L/I/S/T/D/E/N/Q/R/K/P/C/M/F/Y/W	5(12)
₽15	W311G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y	5(12)
in the	F314G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/Y/W	5(14)
####. ##k	W315G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y	5(15)
	E318G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	5(16)
L 4	V322G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(17)
20	F362G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/Y/W	5(17)
jeå. ≅s.	V367G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(19)
	L369G/A/V/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(20)
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	1372G/A/V/L/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(21)
	P374G/A/V/L/I/S/T/D/E/N/Q/R/H/K/C/M/F/Y/W	5(22)
25	D375G/A/V/L/I/S/T/E/N/Q/R/H/K/P/C/M/F/Y/W	5(23)
	A377G/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W	5(24)
	Y378G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W	5(25)
	P382G/A/V/L/I/S/T/D/E/N/Q/R/H/K/C/M/F/Y/W	5(26)
	Y383G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W	5(27)
30	R563G/A/V/L/I/S/T/D/E/N/Q/H/K/P/C/M/F/Y/W	5(28)
	~ · · · · · · · · · · · · · · · · · · ·	J(20)

More specifically, this embodiment relates to an analogue comprising any combination of at least two mutated amino acids, or any one of the above mentioned sequences of mutations, or any separate one amino acid mutation selected from the group consisting of sequences nos 1-9, 13-15, 17-24, 26 and 28, which are all novel mutations that have never been published before the present application. As two specific embodiments of the present mutations according to the invention, E271Q and D375N are mentioned, which have shown to be especially advantageous. However, the other sequences not specified above are novel in the present context and thus such specific uses thereof are within the scope of the present invention.

	Table 6: Mutations of the curved outside of t	the N-terminal domain
	R17 G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W	6(1)
	K19 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(2)
	H20 G/A/V/L/I/S/T/D/N/E/Q/R/K/P/C/M/F/Y/W	6(3)
5	H22 G/A/V/L/I/S/T/D/N/E/Q/R/K/P/C/M/F/Y/W	6(4)
	R24 G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W	6(5)
	D28 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	6(6)
	T33 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(7)
	T35 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(8)
10	G36/A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(9)
	T37 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(10)
	A39 G/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(11)
	T41 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(12)
	Q43 G/A/V/L/I/S/T/D/N/E/R/H/K/P/C/M/F/Y/W	6(13)
15	K63 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(14)
10 11	V65 G/A/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(15)
	N67 G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W	6(16)
46 m/s 2 m/s 1 m/s 2 m/s	N97 G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W	` '
Ų¶	E99 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(17)
20	V101 G/A/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(18)
e Jek	E103 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(19)
	\$105 G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(20)
T.	E107 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(21)
	K153 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(22)
25	T155 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(23)
L	T157 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(24)
	E159 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(25)
	S161 G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(26)
2	D175 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	6(27)
30	E177 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(28)
	T178 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(29)
	D180 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	6(30)
	R186 G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W	6(31)
	I188 G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(32)
35	K190 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(33)
	1192 G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(34)
	K194 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(35)
	Sind via a sind via a sind a s	6(36)
	Table Table 2	
	Table 7: Mutations at the proline r	ach region
40	T359 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(1)
	E358 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	7(2)
	D443 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	7(3)
	A446 G/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(4)
	Y449 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/W	7(5)
45	S450 G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(6)

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P451 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(7)
G452 /A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(7)
L453 G/A/V/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(8)
P454 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(9)
P455 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(10)
1455 CIA MILIOTEDATE O DITURDO A CONTRA	7(11)
1456 G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(12)
K457 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	7(13)
P458 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(14)
N459 G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W	7(15)
Y460 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/W	7(16)
D461 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	7(17)

2.4.5 (d) Nucleic acids encoding the novel compounds

Further, the invention also relates to an isolated nucleic acid encoding a novel analogue as defined above, that is, including a combination of any at least two of said mutations or one of the novel mutations, as well as a nucleic acid capable of specifically hybridising to a such a nucleic acid. The conditions of specific hybridisation are defined above in the section "Definitions". Further, the invention also relates to any vector or carrier comprising such a nucleotide, such as plasmids, viral vectors, e.g. retrovirus, oligonucleotides etc. Thus, any cell including such a nucleic acid or vector are also within the scope of the present invention and may e.g. be a mammalian cell, such as a human cell, or any other eucaryotic cell, or a procaryotic cell, such as a bacterium. The above mentioned elements may be used in the design of model systems useful in the study of the diseases discussed elsewhere in this application, which systems may be cell cultures, animal models, such as mice, etc.

2.4.6 (a) Production and purification of genetically modified forms of LTA₄ hydrolase

Yet another aspect of the present invention is a process for the production of a novel genetically modified form of LTA₄ hydrolase identified or designed according to the present invention. Thus, the present process involves, after conventional steps of insertion a gene encoding the desired product in a host cell and expression thereof, a purification procedure, which includes a hydroxyapatite-based chromatography and a subsequent anion exchange chromatography. These last two steps have been shown to be especially advantageous, in fact, even crucial, for obtaining a

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satisfying purity of the novel LTA₄ hydrolase forms according to the invention. The preceding steps are conventional as disclosed in literature and are easily performed by the skilled in this field.

Thus, in more detail, the invention relates to a method for purification of LTA4 hydrolase comprised of (i) precipitation with ammonium sulphate, followed by (ii) separations on FPLC using anion exchange, hydrophobic interaction, and chromatofocusing resins, essentially as described (Wetterholm A., Medina J.F., Rådmark O., Shapiro R., Haeggström J.Z., Vallee B.L., Samuelsson B. *Biochim. Biophys. Acta.* 1080, 96-102 (1991)). To achieve a purity suitable for crystallography, we used (iii) chromatography on hydroxyapatite, e.g., on a TSKgel HA-1000, Tosohaas, followed by (iv) a step of anion-exchange chromatography on e.g., Mono-Q HR5/5.

Further, example 4 below describes in detail a purification of LTA₄ hydrolase according to the invention. Said example may be generalised to describe further the purification according to the invention.

2.4.6 (b) Purified LTA₄ hydrolase

Further, the invention also relates to an essentially pure form of LTA₄ hydrolase obtained by the process described above.

2.4.7 Identification of LTA₄ hydrolase binding compounds

2.4.7 (a) Method

In yet a further aspect, the present invention relates to a method for screening LTA₄ hydrolase binding compounds complementary to a region, preferably an enzymatically active site, e.g. as defined in Tables 1-3, of the LTA₄ hydrolase molecule, which comprises the steps of

- (a) producing a multiplicity of possible complementary structures and
- 25 (b) selecting a structure represented by a three-dimensional representation, wherein the three-dimensional configuration and spatial arrangement of regions of LTA₄ hydrolase involved in binding remain substantially preserved, which selection is based on the three-dimensional structure of LTA₄ hydrolase and/or LTA₄ hydrolase complexed to an inhibitor thereof, e.g. as defined by the coordinates of Table

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More specifically, the method according to the invention will advantageously be used to select compounds capable of inhibiting epoxide hydrolase activity and/or aminopeptidase activity, LTB₄ receptor antagonists or inhibitors of LTC₄ synthases or inhibitors of any member of the M1 class of metallohydrolases. In one preferred embodiment, general enzyme inhibitors are screened for, which inhibitors are useful in the control of any one of a plurality of enzymatic pathways, wherein a metallohydrolase of the M1 type is participating. These general metallohydrolase inhibitors are herein denoted M1 inhibitors.

Structure-based design of inhibitors

In a further embodiment, the present invention relates to a method of structure-based design of LTA₄ hydrolase inhibitors. Such methods are based on the use of the present coordinates, or preferably the coordinates defining a selected region, as templates in order to synthesize advantageous inhibitors with strong and specific binding properties. More specifically, said method first uses a conventional organic synthesis, alone or combined with combinatorial chemistry, wherein the structure of the product of the synthesis is then further refined by cycles of crystallisation of enzyme and inhibitor, followed by another chemical synthesis, the product of which is again refined, etc.

Example 2 describes such a design, wherein it is noted noted that the removal of an extra carbon atom could yield a compound, which is a better inhibitor than this hydroxamic acid compound. Thus, similar conclusions will be drawn from the present method and result in inhibitors with superior properties compared to any prior art inhibitors.

2.4.7 (b) Identified binding compounds

Further, the present invention also relates to any novel compounds identifiable by the present method. Advantageous and desired properties as well as other features of such compounds, e.g. as inhibitors, is discussed above in relation to complementary compounds, analogues etc. In one preferred embodiment of the invention, such an identified compound is an inhibitor of another M1 enzyme than LTA₄ hydrolase, such as . The medicinal aspects of the present compounds will be discussed below.

Protein engineering

2.4.8 (a) Method

In a further aspect, the present invention relates to a method of engineering a protein, which method comprises the steps of

- -identification of a suitable set of mutation sites based on the structure of LTA₄ hydrolase according to the invention,
 - -generation of a library of genes which contains the suitable sequence variations;
 - -selection of clones encoding a LTA4 analogue with a desired activity;
 - wherein said desired activity is the capability of efficiently producing organic compounds of interest.

The present method is based on recent techniques available for generating large libraries of mutated genes (>1 billion variants) which can be attributed to a selection process of individual genes in the laboratory. Such directed evolution schemes have enormous potential for the design of new proteins, including new substrate specificity for enzymes as well as improving enzyme activities.

Directed evolution, or combinatorial engineering schemes have been successfully applied in evolving RNA molecules with improved binding and catalytic activities (Lorsch and Szostak, 1994). Also binding proteins (and peptides) with good affinities can now routinely be evolved based on a range of different protein folds (Nord et al, 1997). The present methods may be used to perform such a directed evolution of advantageous enzyme activity and specificity and may be performed by someone skilled in this field with reference to the literature, see e.g. O. Kuchner and F. H. Arnold (1997); A. Crameri, S.A. Raillard, E. Bermudez and W.P.C.

Stemmer (1998).) In this context, see also the descriptions provided in US patent no 5 873 082, Noguchi, wherein a list processing system for managing and processing lists of data is disclosed; US patent no 5 869 295, LaBean et al., disclosing methods and materials for producing gene libraries; and US patent no 5 856 928, disclosing a process for gene and protein representation, characterization and interpretation thereof.

In general, major difficulties in this kind of process are to search the sequence space: find the suitable sequence variations for a large but limited number of muta-

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tions (for the same protein fold an immense number of variations can be made e.g. 10 resides protein, 20^{100} variants are in theory possible). It is therefor very important to identify the residues in the protein structure which could effect the activity the most, i.e. the residues near the active site area. Thus, in order to enable a successful performance of a method for engineering proteins with properties relevant in the present field, the data discosed above, more specifically, in Tables 2-4, is crucial.

Further references which are relevent in the context of protein engineering are K. Nord, E. Gunneriusson, J. Ringdahl, S. Stahl, M. Uhlen, P.A. Nygren (1997): "Binding proteins selected from combinatorial libraries of an alpha-helical bacterial receptor domain", *Nature Biotechnology*, 15, 772-777 (1997); R. Lorsch and J.W. Szostak (1994): "In vitro evolution of new ribozymes with polynucleotide kinase activity", *Nature*, 371, 31-36; A. Crameri, S.A. Raillard, E. Bermudez and W.P.C. Stemmer (1998): "DNA shuffling of a family of genes from diverse species accelerates directed evolution", *Nature*, 391, 288-291; and O. Kuchner and F. H. Arnold (1997): "Directed evolution of enzyme catalysts", *Trends in Biotechnology*, 15, 523-530.

In an advantageous embodiment, the present method is used to engineer LTA₄ hydrolase inhibitors and/or analogues. In a specific embodiment of said method, a compound capable of mimicking the suicidal mode of LTA₄ hydrolase catalysis, thus acting as a mechanism-based suicide inhibitor, or otherwise capable of regulating the production of LTB₄ is engineered. In an alternative embodiment, an inhibitor of LTC₄ synthase or an LTB₄ receptor antagonist is designed.

2.4.8 (b) Novel specifically designed proteins

Further, the present invention also relates to any novel protein designed by use of the above described method. Once specified, such proteins may be produced by any conventional method well known to the skilled in this field, some of which are examplified below. In Example 2 below, the binding of hydroxamic acid to LTA4 hydrolase is discussed. Thus, such a modified hydroxamic is one example of a novel inhibitor specifically designed according to the invention, and the resoning in the

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example may be used as a basis for the way of reasoning that is used in the present design.

Accordingly, novel enzymes may be produced, which are capable of any different chemical activity. For example, enzymes capable of novel catalytic properties, enzymes that in turn produce enzymes, etc., may be produced according to the present invention.

2.4.8 (c) Use of genetically modified LTA₄ hydrolase

The invention also encompasses the use of a genetically modified LTA4 hydrolase, obtained by any method according to the invention, with altered catalytic properties, e.g., increased ability to synthesize LTB4. The modified enzyme may thus be used for production of LTB4, or any analogues substances, a biomedical reagent which in turn may be used in, e.g., studies of leukotriene metabolism, induction of chemotaxis, as a reference compound in analysis of leukotrienes etc.

2.4.9 Pharmaceutical applications of the present invention

2.4.9 (a) First medical indication

Further, the invention also encompasses a compound obtainable by the method of screening LTA₄ hydrolase binding compounds, structure-based drug design, or the protein engineering methods described above, and more preferably, said compound for use as a medicament. One specifically advantageous embodiment is the herein disclosed novel M1 inhibitor for use as a medicament.

In an advantageous embodiment, the present compounds are used in the manufacture of a medicament for the treatment and/or prevention of acute and chronic inflammatory disorders, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis and chronic obstructive pulmonary disease (COPD); neoplasias and/or cancer; or disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax. Alternatively, the use may relate to the manufacture of a medicament for the treatment and/or prevention of an inflammatory and/or allergenic disorder, such as bronchial asthma, allergic rhinitis, conjunctivitis etc. Yet an alternative use is in the manufacture of a medicament for the treatment and/or prevention of infection caused be human immunodeficiency virus

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(HIV). The novel M1 inhibitor are preferably used in medicaments for the treatment and/or prevention of such various diseases as cancer and/or endochrinological disturbances.

2.4.9 (b) Second medical indication and pharmaceutical methods

Thus, the present invention relates to the above mentioned molecules prepared by the method according to the invention for use in the manufacture of various medicaments for the above defined conditions. The invention also encompasses pharmaceutical preparations containing these molecules together with pharmaceutically acceptable carriers. Methods for the preparation of pharmaceutical preparations are e.g. found in Remington's Pharmaceutical Sciences, Mack Publishing Company, Philadelphia, PA, 17th ed. (1985). For a review of drug delivery, see Langer, Science 249:1527-1533 (1990). As those skilled in this field easily realise, the form of such a pharmaceutical preparation, the mode of administration thereof as well as suitable dosages will depend on the specific disease to be treated, the nature of the active substance used, the patient's age, body weight etc.

2.4.9 c) Methods of treatment

The present invention also encompasses any method of treatment for the above defined purposes. Exact details regarding such methods are determined by the practitioner depending on the specific circumstances from case to case.

2.5 Production of novel proteinaeous compounds

The compounds, which may be proteins, polypeptides, peptides or any other organic molecules, prepared according to the methods according to the invention may be synthesized chemically by methods well known to those of skill in this field or they may be prepared by use of recombinant DNA technology by any suitable method well known to those of skill in this field. General methods of synthesis are e.g. found in Berger and Kimmel, Guide to Molecular Cloning Techniques, Methods in Enzymology, vol. 152, Academic Press, Inc., San Diego, CA; Sambrook et al., Molecular Cloning, A Laboratory Manual, 2nd Ed., vol. 1-3, Cold Spring Harbor Laboratory, Cold Spring Harbor, NY, 1989; and Current Protocols in Molecular Biology, F.M. Ausbel et al., Current Protocols (1994). Methods of reducing and denaturing proteins and inducing re-folding are well known to those of skill in the art,

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see e.g. Debinski et al., J. Biol. Chem., 268: 14065-14070 (1993); Kreitman and Pastan, Bioconjug. Chem., 4: 581-585 (1993); and Buchner et al., Anal. Biochem., 205: 263-270 (1992).

2. 6 Detailed description of the drawings

5 Figure 1 shows key enzymes and intermediates in leukotriene biosynthesis.

Figure 2 shows 2Fo-Fc density contoured at 1.1 σ. Part of the active site in the neighborhood of the bestatin molecules is shown. Figures are created using a modified version of Molscript48,49.

Figure 3 is a ribbon diagram of the tertiary structure of LTA4 hydrolase. The Nterminal domain at the top of the diagram is rich in β-strands and connects to the catalytic domain to the left in the figure which is more \alpha-helical and extends into the central part of the molecule. The C-terminal domain, illustrated at the bottom of the ribbon diagram, extends towards the right side of the catalytic domain.

Figure 4 (a) is a ribbon diagram of the N-terminal domain with its layers of βstrands, while (b) is a superimposition of the Ca trace of the N-terminal domain on the Cα trace of bacteriochlorophyll a. The N-terminal domain covers approx, half of the bacteriochlorophyll a structure (the right and bottom part of the diagram).

Figure 5 (a) is a ribbon diagram of the catalytic domain. In the center of the diagram, the three zinc binding ligands, His295, His299, and Glu318, as well as the inhibitor bestatin are depicted in ball and stick representation. The zinc ion is shown as a CPK model. The diagram in (b) shows the structure of thermolysin in the same orientation as the catalytic domain of LTA4 hydrolase. The three zinc ligands, His142, His146, and Glu166, as well as the inhibitor Cbz-GlyP-(O)-Leu-Leu50 are depicted in ball-and stick representation. The zinc ion is shown as a CPK model.

25 Figure 6 shows the structure of the C-terminal domain.

> Figure 7 shows the zinc binding ligands in LTA4 hydrolase, His295, His299, and Glu318, superimposed on those in thermolysin, His142, His146, and Glu-166. Other catalytic or neighboring residues in the two enzymes are Tyr383, Glu325, Glu296, Thr302, and Asn317 in LTA4 hydrolase which correspond to His231, Asp170,

30 Glu143, Asn165, and Tyr157 in thermolysin.

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Figure 8 (a) is a Ball-and-Stick presentation of the binding of bestatin in LTA4 hydrolase.

Figure 8 (b) is a schematic overview of bestatin binding in LTA4 hydrolase.

Figure 9 (a) is a wire representation of the cavity found in LTA4 hydrolase (shown as $C\alpha$ -trace).

Figure 9 (b) is a schematic presentation for the proposed binding of LTA4 into the cavity.

Figure 10 is a schematic representation for the proposed epoxide hydrolase reaction mechanism. The catalytic zinc acts as a Lewis acid and activates the epoxide to form a carbocation intermediate according to an SN1 reaction. Water is added at C12 in a stereospecific manner, presumably directed by Asp375. The double bond geometry is controlled by the binding conformation of LTA4. Further details are given elsewhere in the present description.

3. EXPERIMENTAL

The following examples are intended for illustrating purposes only and should not in any way be used to construe the scope of the protection of the present invention as defined by the appended claims. All the references given below, and previously in this specification, are hereby included herein by reference.

3.1 Examples

Example 1: Binding of the thiol-compound (I)

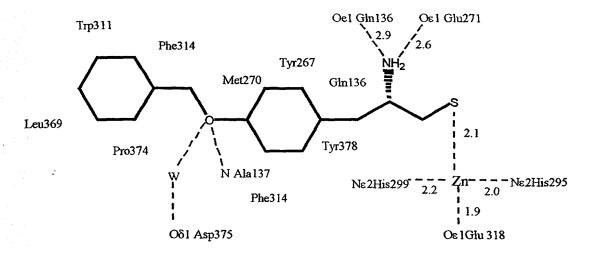
The thiol group of the compound is ligated to the Zn²⁺ ion, that has a tetra-hedral configuration. Both the phenyl-groups are making extensive hydrophobic interactions. The first one makes aromatic stacking interactions with Phe314 and Trp311. Further hydrophobic interactions are made with Pro374 and Leu369. The other phenyl ring is making stacking interactions with Tyr267 and Tyr378. Met270 and Gln136 provide additional hydrophobic interactions. The ether-oxygen in the linker between the two phenyl rings makes a hydrogen bond to the backbone nitrogen of

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Ala137 and also with a water molecule which is linked to Asp375. The amine group makes interactions to the Oa1 of Gln136 and the Oa1 of Glu271.



Formula (I)

Example 2: Binding of the hydroxamic acid compound (II)

The binding of this compound is very similar to the binding of the thiol compound described above. The manner in which the phenyl-moieties, the linker region and the amine group are bound is identical. The manner in which the hydroxamic acid part is bound is different in comparison with other complexes such as thermolysin-HA complexes and LTA₄-hydrolase-bestatin complex. Instead of a double interaction of the hydroxyl and carbonyl oxygens and the Zn ion resulting in a pentavalent co-ordination, here only one of the oxygens (the hydroxyl) is making an interaction with the Zn ion giving a tetrahedral co-ordination. The other oxygens make an interaction to Asp296 and the backbone nitrogen of Gly268. This difference is probably due to the tight binding of the phenyl rings and the amine group. The linkage between the amine group and the hydroxamic acid group contains one more carbon atom than in a normal or modified peptide-linkage. Since the binding site for substrates is rather narrow near the Zn ion, the conformation of compounds which bind in this area is rather restricted. Therefore one of the otherwise binding oxygens is pushed out and can no longer make an interaction with the Zn²⁺ ion. Removal of this extra

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carbon atom could yield a compound which is a better inhibitor than this hydroxamic acid compound. The acid group at the other end of the compound is fixed by making a double interaction with the NE and the Nh2 of Arg563.

Formula (II)

Example 3: Structure determination of two specific inhibitor-LTA₄ hydrolase complexes

Crystals, grown as described above, were soaked in 1 mM solution of thiolamine (Yuan et al., 1993) or 0.5 mM solution of hydroxamic acid (Hogg et al., 1995) in 15% PEG8000, 50 mM Imidazol pH 6.7, 25 mM acetate and 2.5 mM YbCl3. After at least 24 hours, the crystals were transferred to a solution that contained a cryoprotectant (see above) and subsequently flash frozen in liquid nitrogen. The data for the crystal soaked with thiolamine was obtained at BM14B at the EMBL-outstation in DESY, Hamburg. The data for the hydroxamic acid was collected at beamline 7/11 at MAX-lab, Lund. Statistics from the data collections are shown in the table. The data were processed using MOSFLM, merging and other manipulations were performed by programs from CCP4 and the BIOMOL packages. The refinement procedures for both datasets were very similar. First rigid body refinement using TNT was performed. As a starting model for refinement and model building the structure of LTA4 hydrolase complexed with bestatin was used. The bestatin molecule and all water molecules were deleted from the model. After this initial refine-

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ment it was possible to build the inhibitors into the protein. For evaluation of the density maps and model-building the program QUANTA (Molecular Simulations Inc., Burlington, MA) was used. The refinement was continued using TNT and was combined with sessions of model-building. In all rounds no sigma cut-offs were used and the resolution was slowly increased during the procedure. Water molecules were identified and incorporated into the models. During these procedures the Rfree was carefully monitored. When refinement had converged, it was finished with one round in which all reflections, including those who were used for the calculations of the Rfree, were incorporated. Statistics about refinement and quality of the models can be found in Table 5.

Table 8: Statistics of refinement and quality of the model

	Thiolamine (Thiol)	Hydroxamic acid (HA)
Resolution	15-2.5Å	15-1.8Å
Rfactor	17.8%	24.2%
Rfree	24.4	29.7%
Bond Lengths	0.011Å	0.012Å
Angles	1.9°	2.0°
Trigonal groups	0.005Å	0.006Å
Planar groups	0.009Å	0.010Å
Contacts	0.026Å	0.041Å
No. of waters	252	127

Example 4: Purification of LTA4 hydrolase.

For adsorption chromatography on hydroxyapatite, a TSKgel HA-1000 column (Tosohaas) was equilibrated in 10 mM potassium phosphate buffer, pH 7.1, supplemented with 0.2 mM CaCl₂. The enzyme sample was applied and a linear gradi-

ent of increasing phosphate (10 - 400 mM) was developed by mixing the starting buffer with 400 mM potassium phosphate buffer, pH 6.8, supplemented with 10 μM CaCl₂. Active fractions containing LTA4 hydrolase were eluted between 150 - 190

mM potassium phosphate.

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Anion exchange chromatography was performed on a Mono-Q HR 5/5 column (Pharmacia Biotech) equilibrated with the loading buffer 10 mM Tris-Cl, pH 8. The pure protein was eluted using a linear gradient of KCl (0 - 500 mM) and was recovered at 110 - 140 mM KCl.

Example 5: Enzyme engineering

The present inventors have shown, that when Tyr-378 in LTA4 hydrolase was exchanged for a Phe residue, the resulting mutated enzyme was no longer suicide inhibited by LTA4 and exhibited a substantially increased catalytic efficiency. Furthermore, the mutated enzyme was capable of converting LTA4 not only into the natural product LTB4, but also into a novel metabolite, 6-trans-8-cis-LTB4. (Mueller, M.J., et al. Proc Natl Acad Sci U S A 93, 5931-5935 (1996)).

Example 6: Enzyme-engineering

Tyr-383 in mouse LTA4 hydrolase was exchanged for Gln residue, which resulted in a mutated enzyme capable of forming the unnatural product 5S, 6S-dihydroxy-7,9-trans-11,14-cis-eicosatetraenoic acid from LTA4 (Andberg, M., Hamberg, M. & Haeggstrom, J.Z. J. Biol. Chem. 272, 23057-23063 (1997)).

Example 7: Crystallisation of LTA₄ hydrolase

LTA₄ hydrolase was crystallised using YbCl₃ as an additive, 15% PEG and 50 mM Na-acetate as precipitant and 50 mM imidazole, pH 6.7, as buffer. Liquid-liquid-diffusion in capillaries were used as crystallisation set-ups.

3.2 Materials and Methods

Enzyme purification. Human recombinant LTA4 hydrolase was expressed in E. coli and purified to homogeneity in four chromatographic steps on FPLC using anion exchange, hydrophobic interaction, chromatofocusing, and hydroxyapatite resins, essentially as described (Wetterholm A., Medina J.F., Rådmark O., Shapiro R., Haeggström J.Z., Vallee B.L., Samuelsson B. Recombinant mouse leukotriene A4 hyd-

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rolase: a zinc metalloenzyme with dual enzymatic activities. *Biochim. Biophys. Acta.* 1080, 96-102 (1991)).

Crystallization conditions. The chemicals used for the crystallization experiments were purchased from Merck and were of highest purity available. The sparse matrix kit was obtained from Hampton Research. Crystallization conditions for the protein were initially sought by using the sparse matrix approach (Jancarik, J. & Kim, S.-H. J. Appl. Crystallogr. 24, 409-411 (1991)) in hanging drop vapor diffusion set-ups in cell culture plates at room temperature. Under condition 28, (30% PEG8000, 0.2 M sodium-acetate, 0.1 M cacodylate buffer, pH 6.5) needles grew. They were subsequently reproduced and optimized using a finer grid search, different temperatures for the equilibration and testing of additives. Crystals were only obtained when the inhibitor bestatin was present in the crystallization set-ups. Using YbCl3 as an additive and switching to liquid-liquid diffusion in capillaries, allowed plate-like crystals to grow. Thus, 5 µl 28% PEG8000, 0.1 mM Na-acetate, 0.1 mM imidazole buffer, pH 6.8, 5 mM YbCl3 is injected into the bottom of a melting point capillary and an equal volume of LTA4 hydrolase (5 mg/ml) in 10 mM Tris-Cl, pH 8, supplemented with 1 mM bestatin, is layered on top. Finally, the capillary is closed and stored at 22°C. Crystals with an average size of 0.6 x 0.4 x 0.05 mm³ appear in 3 to 4 weeks.

<u>Crystal properties</u>. The plate-like crystals diffract beyond 2Å using synchrotron radiation. They belong to space-group P21212 with cell dimensions a = 67.59 Å, b = 133.51 Å, c = 83.40 Å, $a = b = g = 90 ^{\circ}$ at 100K. As a cryo-solution, a mixture of 15%PEG 8000, 50 mM Na-acetate, 50 mM imidazole buffer, pH 6.8, 2.5 mM YbCl3, and 25% glycerol was used. Assuming one molecule per asymmetric unit the solvent content of the crystals is 48%.

<u>Structure determination</u>. The structure was determined by using multiple anomalous dispersion measurements on the LIII edge of Ytterbium ($\lambda = 1.3862$ Å) at beam line BM14 at the European Synchrotron Radiation Facility (ESRF), Grenoble. Three datasets, peak (PK), point of inflection (PI) and remote (RM), were collected to 2.5Å resolution from the same crystal. The crystal was aligned such that Bijvoet

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equivalent reflections could be collected in one pass of 90° for each wavelength. For RM a subsequent dataset to 2.15Å was collected. A second crystal was used for obtaining a dataset to 1.95Å. (For statistics on data-collection and quality, see table 1). Data were integrated using the program Denzo, scaled to each other using Scalepack (Otwinowski, Z. Data collection and Processing. Proceedings of the ccp4 study weekend. SERC Daresbury Laboratory, Warrington, UK., 56-62 (1993)) and further analyzed using programs from the CCP4 package (Collaborative Computing Project Number 4. Acta Crystallogr. Sect. D 50, 760-763 (1994)).

From Patterson functions one major and one minor Yb position could readily be identified, a third position was identified during heavy atom refinement in difference Fourier maps. The heavy atom parameters were refined using MLPHARE (Otwinowski, Z. Isomorphous replacement anomalous scattering. Proceedings of the CCP4 study weekend. SERC Daresbury Laboratory, Warrington, UK., 80-85 (1991)) and SHARP (de La Fortelle, E. & Bricogne, G. Met. Enzymol. 276, 472-494 (1997)). The final figures of merit was 0.57 to 2.15Å. Phase information was further improved to 2.15Å by solvent flattening using SOLOMON (Abrahams, J.P. & Leslie, A.G.W. Acta Crystallographica D52, 30-42 (1996)) with a solvent content of 43%. The quality of the maps was very good and the entire protein molecule (residue 1-610) could be traced unambiguously. All model building was performed using QUANTA (Molecular simulations). Refinement was started by a run of slowcooling molecular dynamics in XPLOR (Brünger, A.T., Kuriyan, J. & Karplus, M. Science 235, 458-460 (1987)) using the RM dataset to 2.7Å. The three Yb ions were included into the refinement with full occupancy for the first Yb and half occupancy for the two other ions. All subsequent refinement was performed with TNT (Tronrud, D.E., ten Eyk, L.F. & Matthews, B.W. Acta Crystallogr. Sect. A 43, 481-501 (1987)). The same set of reflections (4% of total amount from 25-1.95Å) for the calculation of Rfee (Brünger, A.T. Nature 355, 472-475 (1992)) was maintained throughout all refinement procedures. The resolution was slowly improved by alternating sessions of model-building and refinement. The data for the second crystal to 1.95Å were used for further refinement during which a Zn ion, bestatin, an acetate

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and an imidazole molecule were identified. Judged from the B-factors these molecules are all fully occupied. 540 water molecules were added to the coordinates. The Rfree was 24.7% and the working R-factor was 18.8% for all data between 25-1.95 Å. In a final round of refinement all data between 25-1.95 Å were included, yielding a final R-factor of 18.5 % for residues 1-610, 3 Yb ions, 1 Zn, 1 bestatin, 1 imidazole, 1 acetate and 540 water molecules. Most of the model is in good density (Fig. 2) except a loop encompassing residues 179 to 184 for which only poor density was obtained. The model has good stereo-chemical parameters (r.m.s bonds =0.010Å, r.m.s angles = 2.2°) and 91.7% of the residues lie in the most favored part of the Ramachandran plot.

4. RESULTS AND DISCUSSION

4.1 Overall structure and domain organization

The leukotriene A4 hydrolase molecule is folded into three domains; an N-terminal domain, a catalytic domain and a C-terminal domain which together form a flat triangular arrangement with approximate dimensions of $85 \times 65 \times 50 \text{ Å}^3$. The overall structure of the enzyme is depicted in figure 3. Although the three domains pack closely and make contact with each other, a deep cleft is formed in between.

4.2 The N-terminal domain is structurally related to bacteriochlorophyll a

The N-terminal domain (residue 1-209) is composed of one 7 stranded mixed b-sheet, one 4 and one 3 stranded antiparallel β -sheet. Strands from the larger β -sheet continue into the two smaller β -sheets that pack on the edges of the same side of the larger sheet so that a kind of envelope is formed (Fig. 4a & b). The two small β -sheets are turned towards the inside of the whole protein while the larger β -sheet is exposed to solvent and forms a large concave surface area. Loops connecting the other strands and hydrophobic residues fill the core of this domain. The N-terminal domain of LTA4 hydrolase shares important structural features with the chlorophyll-containing enzyme bacteriochlorophyll (Bchl) α (Matthews, B., Fenna, R., Bolognesi, M., Schmid, M. & Olson, J. J. Mol. Biol. 131, 259-285 (1979)). Thus, 111 C α positions have equivalent positions in the two proteins despite the absence

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of any sequence identity (Fig. 4b). The domain is about half the size of Bchl a

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which has a single domain structure without major extensions. Like Bchl a, the shape of the N-terminal domain resembles an envelope (or Taco) with a hollow inside and in Bchl a, 7 bacteriochlorophylls are buried in this cavity. However, the domain is not as hollow as BChl a since loop 135-155, which contains a small helical segment, is turned inwards and fills up the core. In BChl a the equivalent loop (290–305) is positioned more towards the exterior of the protein, thereby leaving space for some of the tertrapyrroles of the bacteriochlorophylls. The large sheet (17 strands) of Bchl a is truncated to only 7 strands in LTA4 hydrolase. Especially the region between residue 35 and 263 of Bchl a has been replaced by a much shorter region in LTA4 hydrolase (res. 45 to 98) that forms the 3 stranded small B-sheet and the edge strand of the larger 7 stranded β-sheet. The structure of the other half of the molecule is almost completely conserved, except the insertion of two extra strands instead of loops in LTA4 hydrolase. The structural homology between Bchl a, a protein involved in light harvesting, and LTA4 hydrolase was certainly unexpected. In LTA4 hydrolase, the function of the N-terminal domain is not yet known, but one may speculate that it participates in binding to hydrophobic molecules or surfaces with a possible regulatory function. In mammalian 15-lipoxygenase, a similar function was proposed for an N-terminal B-barrel domain with structural homology to a corresponding C-terminal domain in mammalian lipases (Gillmor, S.A., Villasenor, A., Fletterick, R., Sigal, E. & Browner, M.F. Nature Struc. Biol. 4. 1003-1009 (1997)).

The connection from the N-terminal to the catalytic domain is very short, a strand from the 4 stranded β-sheet connects into a strand of a 5-stranded antiparallel β-sheet of the catalytic domain. The two sheets are closely packed and the interface is mainly hydrophobic in character with 14 hydrophobic residues contributing from the N-terminal domain and 11 from the catalytic domain. Hydrogen bonds occur between Gln116 and Ser264, Ser124 and Gln226, the backbone of Ser124 and Glu223, the backbone of Ser151 and Lys309, Lys153 and the backbone of Leu305 and indirectly through a water molecule between Tyr130 and the back-

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bone of Val260. Two salt-bridges between His139 and Asp375 and between Arg174 and Asp257 complete the interactions made in this interface.

4.3 The catalytic domain contains the zinc binding site and is structurally similar to thermolysin

The structure of the catalytic domain (res. 210-450) is surprisingly similar to the structure of thermolysin (Fig. 5a & b) (Holmes, M. & Matthews, B. J. Mol. Biol. 160, 623-639 (1982)). When the amino acid sequence in this domain was compared with that of thermolysin, the sequence identity was found to be very low (essentially confined to the zinc binding motifs). However, the structural homology stretches out over the whole domain. Thus, no less than 146 Ca positions overlap with an r.m.s. deviation of 1.946 Å. Like thermolysin, the catalytic domain consists of two lobes, one mainly a-helical and one mixed a/b lobe. The a-lobe consists of 6 major helices interconnected by long loops containing smaller helical segments, while the a/b lobe has a 5 stranded mixed β-sheet lined with 3 helices on one side. The zinc binding site is found in between the two lobes. Since this domain contains only 245 amino acids and thermolysin contains 314 residues, some truncations have taken place, especially in the a/b lobe in which the N-terminal extended b structure is truncated and only a mixed 5 stranded β-sheet remains. The changes in the a-lobe are smaller. Here the long meandering loop 181 to 221 has been replaced by a long a-helix and the b-hairpin from 245 to 258 has been deleted.

A loop in extended conformation on the surface of the protein from 451 to 463 connects the catalytic domain with the C-terminal domain. Interestingly, this segment contains a highly conserved proline rich motif P451-G-f-P-P-x-K-P-x-Y460 which bears some resemblance to an SH3 domain recognition sequence. However, the canonical arginine residue is not present on either side of the proline motif. Nevertheless, since this stretch of amino acids is exposed on the surface of the protein, it is still possible that it could serve as an anchoring site for protein-protein interactions.

The C-terminal domain (464-610) is composed of 9 a-helices that form an unusual coil of helices reminiscent of the ones found in lytic transglycosylase⁴⁰ and

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recently in the armadillo repeat region of b-catenin (Huber, A.H., Nelson, W.J. & Weis, W.I. Cell 90, 871-882 (1997)) (Fig. 6). The helices pack into two layers of parallel helices (5 inner and 4 outer helices) and in an anti-parallel manner between the two layers. The arrangements found in the two other proteins are much larger and form super-helical structures. In the C-terminal domain of LTA4 hydrolase, the arrangement is more straight and has a very compact shape. One of the helices is deformed and one of the interconnecting loops is long and contains a small 310 helix. The domain makes contacts with both the a-lobe of the catalytic domain and one of the edges of the N-terminal domain. It is positioned in a way such that the helices lie perpendicular to the 7 stranded b-sheet of the N-terminal domain and to most of the helices in the catalytic domain. The helices are amphipatic in character, with the hydrophobic sides towards the middle of the domain and hydrophilic residues pointing towards the solvent and into the deep cleft in the middle of the whole molecule. This side of the cleft is highly polar; 10 Arg and Lys residues and 4 Asp and Glu residues are positioned on this side.

4.4 Zinc coordination

The immediate surroundings of the active site Zn²⁺ ion are very similar in thermolysin and LTA4 hydrolase. The Zn²⁺ is bound between the two lobes and is coordinated by His295, His299, one carboxylic oxygen of Glu318 and the carbonyl and hydroxyl oxygens of the inhibitor bestatin so that a square based pyramid is formed. The two histidines originate from a long a-helix and the glutamate from a neighboring a-helix, all in the a-lobe. Glu296 and Tyr383, two residues implicated in the reaction mechanism for the peptide cleaving activity, are located near the Zn ion. Glu296, the putative general base, is positioned next to the metal ligand His295 and bends over the bestatin molecule and Tyr383, which was described as a proton donor, also makes contact with the bestatin molecule (Figure 8a).

Interestingly, the second layer around the Zn ion shows differences between thermolysin and LTA4 hydrolase. In both enzymes the orientation of the zinc binding ligands is fixed by hydrogen bonds, however the hydrogen bond acceptors are positioned differently. In thermolysin, the Nd1 of His142 is hydrogen bonded to the

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Od2 of Asp170, while in LTA4 hydrolase the Nd1 of His295 is hydrogen bonded to the Oe1 of Glu325. This residue comes from a structural equivalent to the helix carrying Asp170 in thermolysin, but is shifted half a turn outwards. The Nd1 of His146 in thermolysin is hydrogen bonded to the Od1 of Asn165. This residue is part of the zinc binding signature and is conserved between the two enzymes. However, in LTA4 hydrolase the helix in which this conserved residue is placed has been rotated slightly and Asn317 is no longer making a hydrogen bond to His299. The orientation of His299 is now fixed by a hydrogen bond from the Nd1 to the carbonyl backbone oxygen of Thr302. The Od1 of Asn317 makes instead a hydrogen bond to the backbone amide of Asn381 while the Nd2 makes a hydrogen bond to the hydroxyl group of Tyr200. The last protein-ligand, Glu166 is in thermolysin hydrogen bonded to Tyr157 and a water molecule, in LTA4 hydrolase, Glu318 is only hydrogen bonded to a water molecule (Fig. 7).

4.5 Bestatin binding

Although the zinc binding site is formed by residues only from the catalytic domain and most catalytic residues also come from this domain, the active site itself is surrounded by loops from all three domains. The binding of bestatin reflects this, since it makes interactions with residues from all three domains. The main interactions of bestatin are made through the carbonyl and hydroxyl oxygens to the Zn atom. Hydrophobic interactions are made between the phenyl moiety and the phenyl rings of Tyr267, Phe316, Tyr378 and Tyr383. Also, Met270 and Gln136 are involved (Fig. 8a). The other end of the inhibitor is pointing towards the solvent, the leucine moiety makes interactions with Val292 and His295, while the carboxylic oxygens make interactions with Arg563 and Lys565 through water molecules as well as hydrogen bonds to the backbone nitrogen atoms of Gly268 and Gly269. Hydrogen bonds are formed between the peptidyl N of bestatin and Oe2 of Glu296 and between the terminal NH2 and the Oe1 of Glu271 and Oe1 of Gln136. The hydroxyl oxygen makes apart from the interaction with the Zn ion also an interaction to the OH of Tyr383. (For schematic overview see Fig. 8b). Tyr378 which gets modified during suicide inactivation sits slightly further away, but makes a hydro-

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gen bond to Tyr383 and some hydrophobic interactions with the phenyl ring of the inhibitor. These two tyrosine are both found on the same stretch of amino-acids that in thermolysin form a long a helix, however in leukotriene hydrolase this helix is interrupted and two turns of the helix are replaced by three residues (378-380) in an extended conformation. The binding of bestatin is quite different as was found in the complex between bestatin and bovine lens leucine amino-peptidase (blLAP) (Burley, S., David, P., Sweet, R., Taylor, A. & Lipscomb, W. J. Mol. Biol. 224, 113-140 (1992)). In that complex, bestatin was bound to the Zn by both the terminal nitrogen and the nonproteinaceous P1 hydroxyl oxygen, while in LTA4 hydrolase the bestatin is bound by the hydroxyl and carbonyl oxygens. The terminal nitrogen is involved in hydrogen bonding to Glu271 and Gln136. These differences could stem from the fact the blLAP is a bimetal protein with a different reaction mechanism. Moreover the binding of bestatin as seen in LTA4 hydrolase is similar with the complexes formed between thermolysin and hydroxamates which also act as bidentate ligands by the hydroxyl and carbonyl oxygens (Holmes, M. & Matthews, B. Biochemistry 20 (1981)).

Behind the pocket in which the phenyl ring of bestatin binds, there is a cavity that stretches 15 Å deeper into the protein and is approximately 6 to 7 Å wide. In the present structure this cavity is filled with water molecules. It has however a very hydrophobic nature and is lined with Trp311, Phe314, Trp315 Phe362, Leu365, Val367, Leu369, Pro374, Ala377, Tyr378, and Pro382. Most of these residues are strictly conserved or conserved in nature in all LTA4 hydrolase sequences known up until now, with the exception of Val367, which is replaced by a Gln in the yeast and *C. elegans* sequences. Interestingly space for this cavity is partly created by the interruption by the extended conformation in the stretch where Tyr378 and Tyr383 are found. One patch of this binding site is quite hydrophilic with Asn134, Asp375 and the OH of Tyr267 clustering together. This bigger cavity could be a binding site for the LTA4 substrate molecule. If the epoxide moiety would bind in a similar way as the carbonyl oxygen of bestatin to the Zn ion, then the hydrophobic tail would fit snugly into the binding site now occupied by the phenyl group of bestatin and

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would continue into the deeper hydrophobic cavity (Fig. 9a). The other tail would sit in the pocket that is now occupied by the carboxy group of bestatin and it would be long enough for the carboxylic acid to make direct electrostatic interactions with the conserved Arg563 and Lys565.

The replacement of Val367 by Gln as seen in the enzyme from yeast would make the hydrophobic channel shorter and this might be one of the reasons why the yeast enzyme has a poor leukotriene A4 epoxide hydrolase activity. The manner in which the leukotriene molecule would bind is similar as what is proposed for binding of arachidonic acid in 15-lipoxygenase (Gillmor, S.A., Villasenor, A., Fletterick, R., Sigal, E. & Browner, M.F. *Nature Struc. Biol.* 4, 1003-1009 (1997)) with the hydrophobic end buried inside the protein and the carboxylic acid more towards the surface making interactions with Arg and Lys residues.

The binding of bestatin acts also as a guide for the binding of peptide substrate molecules. From systematic binding studies with tri-peptides it was shown that the enzyme has a strong preference for an arginine residue as the N-terminal residue and for several tri-peptides the enzyme has a kcat/Km ratio 10-fold the kcat/Km for LTA4 (Örning, L., Gierse, J.K. & Fitzpatrick, F.A. J. Biol. Chem. 269, 11269-11273 (1994). If we roughly model a peptide in the active site with an N-terminal Arg with the carbonyl oxygen sitting on the place of the hydroxyl group of bestatin, then the Arg side-chain of this residue would sit in the same place as the phenyl group of the bestatin with the guanidinium headgroup interacting with the conserved Asp375 and the OH of Tyr267 and the more hydrophobic Cb, Cd and Cg atoms making similar interactions as the phenyl ring. The terminal aminogroup could make the same electrostatic interaction as the terminal aminogroup of bestatin with Asp271 and Gln136. This mode of binding of bestatin is in contrast with the mode proposed by Örning, since the phenyl ring seems to occupy the S1 pocket. We also propose that the LTA4 substrate molecule is occupying all three pockets, S1, S'1 and S'2.

If the binding mode of peptides in LTA4 hydrolase is compared with the one described for thermolysin, a number of differences are observed. In thermolysin, the

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peptide molecule is held in place by many interactions to the main chain atoms provided by Asn112, Ala203, Arg203 and Trp115. None of these residues or equivalent residues can be found in the binding site in LTA4 hydrolase. Furthermore, although binding pockets S1 and S'1 are at similar positions as in thermolysin, site S'2 has to be different since its space is occupied by Tyr378 in LTA4 hydrolase. Glu271 and Gln136 and the N-terminal domain are filling up the space into which in thermolysin the upstream peptide binds contributing to the exo-peptidase function instead of an endo-peptidase function as in thermolysin.

4.6 Putative Phosphorylation site

Recently specific phosphorylation by a yet unknown specific kinase of Ser415 has been described as means of regulation of LTA4 hydrolase activity in endothelial cells (Rybina, I.V., Liu, H., Gor, Y. & Feinmark, S.J. *J Biol Chem* 272, 31865-71 (1997)). This residue is conserved in all mammalian LTA4 hydrolases and is embedded in a highly homologous stretch of residues. Phosphorylation of this residue seems to inhibit the epoxide hydrolase activity but not the amino-peptidase activity. In the structure this residue is located in a loop connecting two a-helices that lie on the surface of the molecule. The loop itself is located at the back of the enzyme.

4.7 Aminopeptidase activity

The amino-peptidase activity catalyzed by this enzyme has been well studied and many of the important residues have been target for site-directed mutagenesis work. This lead to a proposal in which Glu296 would act as a general base (Wetterholm, A., et al. Proc Natl Acad Sci U S A 89, 9141-9145 (1992)) and Tyr383 as a putative proton donor (Blomster, M., Wetterholm, A., Mueller, M.J. & Haeggström, J.Z. Eur. J. Biochem. 231, 528-534 (1995)). In the current complex, these residues are involved in hydrogen bonds with the bestatin molecule. If bestatin binding is seen as a rough analog for the transition state binding, then the interaction of Glu296 with the hydroxyl oxygen of bestatin indicates that this residue could indeed activate a water-molecule for the nucleophilic attack. The role of Tyr383 cannot so easily be confirmed, however its position strongly suggest the role of proton donor. In thermolysin the proton donor is His231 and although the Ca position of this resi-

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due is 4.1Å removed from the Ca position of Tyr383 in LTA4 hydrolase, the Nd1 is only 1 Å removed from the OH position of Tyr383. The conserved Glu271 could be involved in the exo-protease activity of the protein. Recently, the analogous Glu350 in aminopeptidase N and Glu352 in aminopeptidase A were subject to site-directed mutagenesis work (Luciani, N., et al. Biochemistry 37, 686-692 (1998); and Vazeux, G., Iturrioz, X., Corvol, P. & Llorenz-Cortez, C. Biochem. J. 334, 407-413 (1998)) and it was observed that mutations of this residue lead to large decreases in the activity in the case of substitutions by conserved amino-acids such as aspartate and glutamine and absence of activity in substitution by alanine. It was concluded that Glu350 belonged to the anionic binding site in that protein. A mechanism based on thermolysin was proposed for aminopeptidase N with a pentavalent transition state with an additional interaction between the free a-aminogroup and Glu350. In this structure we can observe such an interaction between Glu271 and the free aminogroup of bestatin. Furthermore the penta-valent coordination of Zn by the His295, His299, Glu318 and the carbonyl and hydroxyl groups of bestatin indicates that this is an equivalent transition state analog complex as determined previously for thermolysin.

From careful sequence alignments and structural insight we can conclude that the enzymes in the M1 family of proteases will share a highly conserved catalytic domain that includes part of the N-terminal domain as we see it in LTA4 hydrolase and the thermolysin-like domain. There is no homology for residues in the C-terminal domain and we believe that this domain is unique for LTA4 hydrolases. According to the present invention, it is suggested that all proteases belonging to class M1 with the signature HExxH and a Glu 18 residues downstream will function in a similar way to thermolysin.

4.8 Epoxide hydrolase activity

Concerning the epoxide hydrolase activity, much less is known about the functional elements and mechanisms of catalysis. In fact, the prosthetic zinc is the only critical component identified thus far and may potentially assist in the introduction of a water molecule at C12 or in the activation of the epoxide. Although Tyr378 and

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Tyr383 are important active side residues, none of them is essential for catalysis. A mutation of Tyr378 to Phe protects the enzyme against suicide inhibition, however the specificity of the double bond configuration is partly lost (Mueller, M., Andberg, M., Samuelsson, B. & Haeggstrom, J. J. Biol. Chem. 271, 24345-24348 (1996)) since a novel metabolite with a cis-trans-cis conjugated system can be detected. Thus, Tyr378 is a major binding site for LTA4 during suicide inactivation and seems to play a role for the formation of the correct double bond geometry in the product LTB4. Mutations of Tyr383 abolish the amino-peptidase activity where it has a role as potential proton donor (vide supra) but the epoxide hydrolase activity is only decreased compared to wild-type. It is however implicated in the stereospecific introduction of water during the hydrolysis of LTA4 to LTB4 since these mutants convert LTA4 in both LTB4 and 5 [S],6 [S]-DHETE (Andberg, M., Hamberg, M. & Haeggstrom, J. J. Biol. Chem. 272, 23057-23063 (1997)). Moreover careful analysis of the catalytic properties of enzymes mutated in pos. 383, viz [Y383F], [Y383H] and [Y383Q]LTA4 hydrolase have indicated that the epoxide hydrolase reaction follows an SN1 mechanism.

If one considers the chemistry carried out by LTA4 hydrolase, the enzyme has two major tasks during the hydrolysis of LTA4 to LTB4. First introduction of a water molecule stereospecific at C12 and second to generate a cis-double bond Æ6 in the resulting conjugated triene system [cf. Fig. 1]. If LTA4 is modeled into the putative substrate binding pocket as indicated in figure 9b, the catalytic zinc gets close to the epoxide and not C12 of the substrate. Therefore the most likely role of the Zn ion is to act directly as a Lewis acid to activate and open the epoxide ring. This would generate a carbocation, whose charge will be delocalised over the conjugated triene system from C7 to C12. Since this intermediate has an sp2 hydridized planar configuration at C12, it is in principle open for nucleophilic attack from either side of the molecule. The conserved Asp375 is positioned in such a way that a water molecule bound to it is in "attacking" distance of C12 of a modeled LTA4 molecule, the position into which a hydroxyl group is inserted during the reaction.

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This will account for the proper stereo-chemical and positional insertion of the hydroxyl-group at C12 in R configuration.

The shape and curvature of the LTA4 binding pocket also gives a clue as to how the enzyme creates the cis double bond at Æ6. Since there is free rotation between the c6 and c7 of LTA4, this bond may be kept in a "pro-cis" configuration in the transition state, which in turn would facilitate the formation of a Æ6-cis double bond form the carbocation intermediate. If LTA4 is modeled in this way, the entire molecule adopts a bent shape, fitting very well with the architecture of the binding pocket (Fig. 9b). Hence, the critical double bond geometry at Æ6 of LTB4 is probably guaranteed by the exact binding conformation of LTA4 at the active side which in turn is governed by all the structural elements participating in substrate binding. including the carboxylate recognition sites, Arg56 and Lys565, the catalytic zinc and the hydrophobic residues lining the pocket. The putative binding cleft for the leukotriene molecule is narrow and bend and thereby favoring LTA4 over other epoxides. The two tyrosines are positioned such that they are in contact with the triple double bond configuration of a modeled LTA4 molecule at the bent of the putative binding pocket and they are hydrogen-bonded to each other. Therefore their position is ideal for guidance in stereo-specificity of the double bond configuration. The loss of specificity for the hydroxyl-incorporation at the C12 position in case of the Tyr383 position can be explained that mutations at this position would possibly create extra space for a water molecule that could attack at the C6 position and thereby form 5 [S],6 [S]-DHETE.

The position of Tyr378 is such that it is in contact with the C6 atom of the modeled LTA4 molecule. If after opening of the epoxide ring the hydroxyl group of Tyr378 instead of a water molecule would attack the carbon-cation at the C6 position, a covalently attached molecule is formed which forms the suicide inhibited complex. In order to check this hypothesis and to obtain more information about the binding-site for leukotriene A4, the structure of this inhibited species would be essential.

In order to exclude the possibility that residues near the active site might have further catalytic roles in the epoxide hydrolase reaction, a thorough investigation of these residues, such as Glu271 and Gln136 has to be started. Furthermore the proposed role of Asp375 in activating a water molecule for the stereospecific attack at C12 has to be investigated.

Accordingly, the present invention has solved the first specific leukotriene converting enzyme, which for the first time reveals the binding mode for leukotriene molecules. Furthermore, insight is provided in a unique active site that harbours two activities using different amino-acids to catalyze different reactions.

5. CONFORMATIONAL DATA

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Table 9: Structure coordinates of LTA₄ hydrolase-thiolamine complex

.52 50.	activities using different amino-acids to catalyze different reactions.												
25 T.			0				o to vatas	.yze unite	One react	10113.			
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42	<u>5. CONI</u>	FOR	MAT	ION A	4 T	DATA							
 - 4							CT TD						
15	1	aute	<u>9. Su</u>	uctu	16	coordinate	SOILIA	<u>1₄ hydrola</u>	<u>se-thiola</u>	mine complex			
5 FF% -	CRYST	68.	560	132	. 1	50 83.2	70 90.0	90.00	90 00	P21212			
UT	SCALE1		0.0	1459		0.00000	0.0000		0.00000				
15	SCALE2			0000		0.00757	0.0000		0.00000				
#	SCALE3		0.0	0000		0.00000	0.0120		0.00000				
ļ.								_					
			Atom	res	. (Chain No.	x	У	z	occ B-factor			
20		_											
[20	ATOM	1	N	PRO		1	-0.593	16.387	63.494	1.00 97.99			
ing mil. 	MOTA	2	CA	PRO		1	-1.890	16.918	63.874	1.00 97.22			
10 m	MOTA	3	C	PRO		1	-2.210	18.371	63.525	1.00100.00			
]=4 ,	MOTA	4 5	0	PRO		1	-2.402	18.667	62.342	1.00100.00			
. 25	ATOM ATOM		CB	PRO		1	-2.130	16.551	65.332	1.00 97.81			
. 23	ATOM	6 7	CG CD	PRO		1	-1.221	15.355	65.583	1.00100.00			
	ATOM	8	N	PRO GLU		1 2	-0.290	15.233	64.369	1.00 97.05			
	MOTA	9	CA	GLU		2	-2.216	19.272	64.556	1.00 96.95			
	MOTA	10	C	GLU		2	-2.569	20.678	64.314	1.00 95.71			
30	MOTA	11	ŏ	GLU		2	-2.188 -2.512	21.701	65.386	1.00 94.33			
	ATOM	12	СВ	GLU		2	-2.312 -4.105	21.542 20.768	66.562	1.00 93.21			
	ATOM	13	CG	GLU		2	-4.587	21.732	64.214	1.00 97.26			
	ATOM	14	CD	GLU		2	-4.351	21.732	63.125 61.767	1.00100.00			
	ATOM	15		GLU		2	-3.301	21.261	61.152	1.00100.00			
35	MOTA	16		GLU		2	-5.361	20.398	61.368	1.00100.00 1.00100.00			
	ATOM	17	N	ILE		3	-1.550	22.799	64.944	1.00100.00			
	ATOM	18	CA	ILE		3	-1.148	23.905	65.820	1.00 81.53			
	ATOM	19	С	ILE	Α	3	-2.006	25.154	65.661	1.00 75.68			
40	ATOM	20	0	ILE	Α	3	-2.835	25.288	64.763	1.00 76.97			
40	ATOM	21	CB	ILE		3	0.308	24.324	65.707	1.00 83.45			
	MOTA	22		ILE		3	0.452	25.521	64.759	1.00 83.63			
	ATOM	23	CG2	ILE	Α	3	1.198	23.160	65.300	1.00 84.76			
	ATOM	24		ILE		3	-0.184	25.361	63.375	1.00 91.36			
AF	ATOM	25	N	VAL		4	-1.725	26.099	66.523	1.00 61.54			
45	ATOM	26	CA	VAL		4	-2.477	27.303	66.482	1.00 56.32			
	ATOM	27	С	VAL		4	-1.658	28.552	66.623	1.00 50.98			
. ,	ATOM	28	0	VAL		4	-0.803	28.694	67.512	1.00 47.84			
	ATOM	29	CB	VAL		4	-3.514	27.318	67.595	1.00 58.99			
50	ATOM	30		VAL		4	-3.735	28.754	68.047	1.00 58.40			
20	ATOM ATOM	31		VAL		4	-4.819	26.691	67.131	1.00 58.56			
	ATOM	32 33	N CA	ASP		5	-2.012	29.486	65.732	1.00 39.38			
	AIOM	33	CA	ASP	А	5	-1.403	30.782	65.763	1.00 32.64			

		ATOM	34	С	ASP A	5	-2.308	31.596	66.634	1.00 36.35
*		ATOM	35	ŏ	ASP A	5		32.051	66.171	1.00 38.30
		ATOM	36	СВ	ASP A	5		31.492	64.400	1.00 30.30
		ATOM	37	CG	ASP A	5		32.581	64.563	1.00 30.75
	5		38		ASP A	5		33.123	65.635	1.00 25.90
	J .	MOTA			ASP A					
		MOTA	39			5		32.831	63.493	1.00 29.81
		ATOM	40	N	THR A	6		31.745	67.903	1.00 32.32
		MOTA	41	CA	THR A	6		32.507	68.842	1.00 32.08
	10	ATOM	42	C	THR A	6		34.011	68.557	1.00 40.63
	10	ATOM	43	0	THR A	6		34.759	69.132	1.00 46.68
		MOTA	44	CB	THR A	6		32.171	70.295	1.00 44.71
		MOTA	45		THR A	6		32.322	70.505	1.00 51.05
		ATOM	46	CG2	THR A	6	-2.789	30.741	70.604	1.00 35.79
		MOTA	47	N	CYS A	7	-1.842	34.480	67.656	1.00 32.51
	15	MOTA	48	CA	CYS A	7	-1.797	35.923	67.335	1.00 28.92
		ATOM	49	С	CYS A	7	-2.627	36.329	66.129	1.00 31.49
		ATOM	50	0	CYS A	7	-2.780	37.523	65.875	1.00 25.42
		ATOM	51	CB	CYS A	7	-0.362	36.410	67.107	1.00 27.38
		ATOM	52	SG	CYS A	7	0.686	35.944	68.518	1.00 32.02
43	20	ATOM	53	N	SER A	8	-3.140	35.315	65.383	1.00 34.03
u"		ATOM	54	CA	SER A	8	-3.940	35.508	64.158	1.00 32.97
SERVICE SERVICE		ATOM	55	С	SER A	8	-5.410	35.136	64.264	1.00 33.52
2000 2000		ATOM	56	ō	SER A	8	-5.744	34.137	64.866	1.00 32.89
182 770		ATOM	57	СВ	SER A	8	-3.363	34.754	62.980	1.00 34.07
を の の の の の の の の の の の の の	25	ATOM	58	OG	SER A	8	-4.017	35.182	61.798	1.00 34.07
	23	ATOM	59	N	LEU A	9	-6.289	35.921	63.635	1.00 30.03
44 .					LEU A	9	-7.724	35.649		
		ATOM	60	CA					63.672	1.00 31.91
#		ATOM	61	C	LEU A	9	-8.198	35.009	62.377	1.00 36.07
= #/ ₂	20	ATOM	62	0	LEU A	9	-9.359	34.626	62.216	1.00 38.61
T.	30	ATOM	63	CB	LEU A	9	-8.514	36.958	63.874	1.00 32.47
7.		ATOM	64	CG	LEU A	9	-8.306	37.688	65.212	1.00 35.39
		ATOM	65		LEU A	9	-9.113	38.983	65.193	1.00 32.27
- 1522 Mg/		ATOM	66.		LEU A	9	-8.746	36.816	66.397	1.00 33.25
in the	-	ATOM	67	N	ALA A	10	-7.273	34.933	61.443	1.00 28.63
4.	35	MOTA	68	CA	ALA A	10	-7.545	34.408	60.147	1.00 27.14
		MOTA	69	С	ALA A	10	-7.643	32.921	60.090	1.00 34.34
		MOTA	70	0	ALA A	10	-7.296	32.173	61.005	1.00 37.34
		MOTA	71	CB	ALA A	10	-6.551	34.936	59.100	1.00 27.72
		ATOM	72	N	SER A	11	-8.130	32.503	58.959	1.00 32.08
	40	ATOM	73	CA	SER A	11	-8.256	31.115	58.708	1.00 32.03
		ATOM	74	С	SER A	11	-6.838	30.519	58.656	1.00 32.67
		ATOM	75	0	SER A	11	-5.927	31.028	57.986	1.00 29.29
		ATOM	76	CB	SER A	11	-9.013	30.934	57.401	1.00 38.42
		MOTA	77	OG	SER A	11	-10.391	30.728	57.648	1.00 44.17
	45	ATOM	78	N	PRO A	12	-6.651	29.440	59.387	1.00 29.14
		ATOM	79	CA	PRO A	12	-5.370	28.786	59.476	1.00 26.83
		ATOM	80	c	PRO A	12	-4.935	28.176	58.173	1.00 32.64
		ATOM	81	Ō	PRO A	12	-5.737	28.007	57.284	1.00 35.89
		ATOM	82	СВ	PRO A	12	-5.544	27.698	60.540	1.00 28.28
	50	ATOM	83	CG	PRO A	12	-7.029	27.571	60.843	1.00 32.92
		ATOM	84	CD	PRO A	12	-7.731	28.587	59.952	1.00 30.42
		ATOM	85	N	ALA A	13	-3.645	27.836	58.063	1.00 30.42
		MOTA	86	CA	ALA A	13	-3.066	27.236	56.855	
										1.00 28.36
	55	ATOM	87	C	ALA A	13	-3.644	25.852	56.576	1.00 33.99
	55	ATOM	88	0	ALA A	13	-3.455	25.240	55.528	1.00 31.60
		ATOM	89	CB	ALA A	13	-1.561	27.133	57.050	1.00 27.68
		ATOM	90	N	SER A	14	-4.338	25.352	57.571	1.00 31.10
		ATOM	91	CA	SER A	14	-4.919	24.069	57.469	1.00 30.66
	60	MOTA	92	С	SER A	14	-6.242	24.133	56.753	1.00 37.86
	60	ATOM	93	0	SER A	14	-6.768	23.118	56.328	1.00 45.79
		ATOM	94	CB	SER A	14	-5.005	23,386	58.825	1.00 34.33
		MOTA	95	OG	SER A	14	-6.006	23.978	59.621	1.00 41.01
		ATOM	96	N	VAL A	15	-6.785	25.327	56 .6 30	1.00 32.80
		ATOM	. 97	CA	VAL A	15	-8.036	25.529	55.917	1.00 31.81

	MOTA	98	С	VAL A	15	-7.777	26.107	54.507	1.00 34.70
	ATOM	99	Ö	VAL A	15		25.576	53.494	1.00 34.70
	ATOM	100	CB	VAL A	15		26.336	56.720	1.00 31.90
	ATOM	101		VAL A	15		26.638	55.861	1.00 33.31
5	MOTA	102		VAL A	15		25.538	57.949	1.00 30.32
,	ATOM	103	N	CYS A	16		27.183	54.453	1.00 33.85
	ATOM	104	CA	CYS A	16		27.826	53.189	1.00 38.27
	ATOM	105	C	CYS A	16		28.388	53.265	1.00 37.14
	ATOM	106	ō	CYS A	16		28.534	54.322	1.00 39.70
10	ATOM	107	СВ	CYS A	16		28.870	52.581	1.00 42.09
	ATOM	108	SG	CYS A	16		30.418	53.540	1.00 47.38
	ATOM	109	N	ARG A	17		28.722	52.132	1.00 32.10
	MOTA	110	CA	ARG A	17		29.262	52.101	1.00 32.54
	ATOM	111	С	ARG A	17		30.307	51.005	1.00 34.56
15	ATOM	112	0	ARG A	17	-3.511	30.065	49.842	1.00 35.07
	MOTA	113	CB	ARG A	17		28.152	51.758	1.00 36.83
	ATOM	114	CG	ARG A	17	-1.779	27.391	52.915	1.00 40.61
	ATOM	115	CD	ARG A	17	-1.472	25.970	52.503	1.00 27.18
#7s	MOTA	116	NE	ARG A	17	-1.963	25.026	53.501	1.00 52.41
20	ATOM	117	CZ	ARG A	17	* -1.244	24.036	54.035	1.00 69.41
13 20	ATOM	118		ARG A	17		23.812	53.683	1.00 54.86
ul)	MOTA	119	NH2	ARG A	17		23.246	54.952	1.00 49.68
 - 4.	ATOM	120	N	THR A	18		31.454	51.378	1.00 27.06
military	ATOM	121	CA	THR A	18		32.477	50.428	1.00 26.12
25	MOTA	122	С	THR A	18		32.110	49.653	1.00 30.83
UT	ATOM	123	0	THR A	18		31.964	50.194	1.00 29.06
1=4x	MOTA	124	СВ	THR A	18		33.810	51.134	1.00 34.27
562	MOTA	125	OG1		18		34.261	51.738	1.00 32.95
30	ATOM	126	CG2		18		34.839	50.156	1.00 35.91
##3U	ATOM	127	N	LYS A	19		31.955	48.365	1.00 31.55
	MOTA	128	CA	LYS A	19		31.615	47.511	1.00 31.74
n.	ATOM	129	C	LYS A	19 19		32.848	46.906 46.520	1.00 33.90
	ATOM	130 - 131	O CB	LYS A LYS A	19		32.834 30.697	46.320	1.00 34.57
35	MOTA MOTA	132	CG	LYS A	19		29.368	46.924	1.00 36.08 1.00 62.54
JJ	ATOM	133	CD	LYS A	19		28.257	47.057	1.00 82.34
	MOTA	134	CE	LYS A	19		27.880	48.496	1.00 32.23
	ATOM	135	NZ	LYS A	19		27.849	48.745	1.00 55.63
	ATOM	136	N	HIS A	20		33.928	46.810	1.00 31.40
40	MOTA	137	CA	HIS A	20		35.122	46.198	1.00 29.22
	ATOM	138	С	HIS A	20		36.345	46.517	1.00 34.68
	ATOM	139	0	HIS A	20	-1.833	36.239	46.846	1.00 35.34
	ATOM	140	CB	HIS A	20		34.956	44.666	1.00 26.47
	ATOM	141	CG	HIS A	20	0.865	36.022	43.970	1.00 26.77
45	ATOM	142	ND1	HIS A	20	2.249	36.046	43.980	1.00 28.92
	MOTA	143		HIS A	20		37.091	43.280	1.00 27.43
	ATOM	144		HIS A	20		37.126	43.301	1.00 28.21
	ATOM	145	NE2	HIS A	20		37.781	42.865	1.00 28.18
	MOTA	146	N	LEU A	21		37.492	46.390	1.00 30.14
50	MOTA	147	CA	LEU A	21		38.782	46.610	1.00 31.02
	ATOM	148	C	LEU A	21	-0.134	39.786	45.562	1.00 38.34
	ATOM	149	0	LEU A	21		39.952	45.312	1.00 37.30
	MOTA	150	CB	LEU A	21		39.363	47.999	1.00 31.30
55	ATOM	151 152	CG	LEU A	21		40.880	48.047	1.00 32.33
))	ATOM ATOM	152		LEU A	21 21		41.192 41.522	48.324 49.100	1.00 27.10
	ATOM	154	N N	HIS A	22		41.522	44.951	1.00 32.86 1.00 35.47
	ATOM	155	CA	HIS A	22		41.452	43.920	1.00 35.47
	ATOM	156	C	HIS A	22		42.742	44.550	1.00 34.24
60	ATOM	157	o	HIS A	22		42.957	44.905	1.00 35.72
	ATOM	158	CB	HIS A	22		41.244	42.624	1.00 33.72
	ATOM	159	CG	HIS A	22		42.256	41.615	1.00 35.97
	ATOM	160		HIS A	22		42.576	41.384	1.00 38.81
	ATOM	161		HIS A	22		43.043	40.830	1.00 39.07

		1.00	~		00				
	MOTA	162		HIS A	22	-0.019	43.534	40.462	1.00 38.66
	ATOM	163		HIS A	22	-1.262	43.829	40.103	1.00 39.13
	ATOM	164	N	LEU A	23	-0.235	43.539	44.757	1.00 30.17
_	ATOM	165	CA	LEU A	23	-0.416	44.793	45.405	1.00 33.32
: 5	MOTA	166	С	LEU A	23	-0.203	45.949	44.440	1.00 44.46
	ATOM	167	0	LEU A	23	0.828	46.068	43.761	1.00 44.06
	MOTA	168	CB	LEU A	23	0.446	44.882	46.680	1.00 33.72
	MOTA	169	CG	LEU A	23	-0.141	45.682	47.871	1.00 33.15
	ATOM	170	CD1	LEU A	23	0.780	46.835	48.172	1.00 26.07
10	ATOM	171	CD2	LEU A	23	-1.539	46.213	47.609	1.00 35.39
	ATOM	172	N	ARG A	24	-1.256	46.765	44.395	1.00 42.83
	ATOM	173	CA	ARG A	24	-1.406	47.964	43.596	1.00 41.79
	ATOM	174	С	ARG A	24	-1.930	49.005	44.562	1.00 39.15
	ATOM	175	0	ARG A	24	-3.025	48.859	45.107	1.00 39.85
15	ATOM	176	CB	ARG A	24	-2.458	47.716	42.504	1.00 46.35
	ATOM	177	CG	ARG A	24	-2.054	46.750	41.382	1.00 50.50
	ATOM	178	CD	ARG A	24	-2.754	47.058	40.043	1.00 80.27
	ATOM	179	NE	ARG A	24	-4.200	46.798	40.062	1.00 95.12
Party	ATOM	180	CZ	ARG A	24	-5.152	47.703	39.826	1.00100.00
20	ATOM	181		ARG A	24	-4.863	48.973	39.483	1.00100.00
- 4R	MOTA	182		ARG A	24	-6.432	47.326	39.865	1.00100.00
4D	MOTA	183	N	CYS A	25	-1.164	50.028	44.844	1.00100.00
 - -	ATOM	184	CA	CYS A	25	-1.698	50.969	45.813	1.00 32.39
FERN FERN	ATOM	185	C	CYS A	25	-1.061	52.325	45.724	1.00 33.30
25	ATOM	186	0	CYS A	25	-0.012	52.514	45.076	1.00 34.82
	ATOM	187	СВ	CYS A	25	-1.503	50.440	47.257	1.00 31.03
\$= \$\(\)	MOTA	188	SG	CYS A	25	0.231	50.529	47.798	1.00 34.67
		189	N	SER A	26	-1.711	53.257		
188	MOTA ATOM	190	CA	SER A	26	-1.196	54.601	46.418 46.437	1.00 34.39 1.00 36.77
30			CA	SER A	26	-0.963	55.133		
	ATOM	191 192	Ö		26	-1.738		47.821	1.00 39.85
	ATOM	193	СВ	SER A	26		54.853	48.757	1.00 37.56
	ATOM					-1.889	55.600	45.530	1.00 42.70
तिक स्तरि शुक्त सम्बद्ध	ATOM	194	OG	SER A	26	-0.899	56.330	44.824	1.00 61.74
25	ATOM	195	N	VAL A	27	0.133	55.897	47.886	1.00 39.43
↓ 35	ATOM	196	CA		27	0.624	56.583	49.081	1.00 41.31
	ATOM	197	C	VAL A	27	0.209	58.043	49.082	1.00 44.32
•	ATOM	198	0	VAL A	27	0.562	58.799	48.187	1.00 45.24
	ATOM	199	CB	VAL A	27	2.135	56.531	49.207	1.00 46.35
40	ATOM	200		VAL A	27	2.524	57.207	50.522	1.00 45.62
40	ATOM	201		VAL A	27	2.592	55.079	49.178	1.00 47.20
	ATOM	202	N	ASP A	28	-0.553	58.417	50.093	1.00 37.94
	ATOM	203	CA	ASP A	28	-1.040	59.764	50.237	1.00 35.28
	ATOM	204	C	ASP A	28	-0.595	60.366	51.538	1.00 33.85
15	ATOM	205	0	ASP A	28	-1.181	60.099	52.598	1.00 28.52
45	ATOM	206	CB	ASP A	28	-2.559	59.807	50.189	1.00 37.09
	ATOM	207	CG	ASP A	28	-3.055	61.205	50.095	1.00 55.20
	ATOM	208	ODI	ASP A	28	-2.611	62.119	50.767	1.00 59.17
	ATOM	209		ASP A	28	-3.993	61.335	49.192	1.00 61.41
50	MOTA	210	N	PHE A	29	0.436	61.174	51.405	1.00 36.42
50		211	CA	PHE A	29	1.044	61.888	52.512	1.00 43.07
	ATOM	212	C	PHE A	29	0.105	62.928	53.077	1.00 51.14
	ATOM	213	0	PHE A	29	0.161	63.279	54.257	1.00 51.35
	ATOM	214	CB	PHE A	29	2.410	62.517	52.143	1.00 47.77
<i>55</i>	ATOM	215	CG	PHE A	29	3.519	61.485	52.079	1.00 50.86
55		216		PHE A	29	4.066	60.957	53.247	1.00 52.08
	MOTA	217		PHE A	29	3.996	61.001	50.863	1.00 53.94
	MOTA	218		PHE A	29	5.075	59.995	53.215	1.00 52.83
	ATOM	219		PHE A	29	5.013	60.046	50.813	1.00 56.46
	ATOM	220	CZ	PHE A	29	5.559	59.538	51.992	1.00 53.39
60		221	N	THR A	30	-0.766	63.420	52.220	1.00 47.10
	ATOM	222	CA	THR A	30	-1.718	64.386	52.654	1.00 45.48
	ATOM	223	С	THR A	30	-2.788	63.715	53.509	1.00 48.41
	MOTA	224	0	THR A	30	-3.045	64.082	54.649	1.00 48.64
•	MOTA	225	CB	THR A	30	-2.283	65.097	51.434	1.00 54.06

	MOTA	226	OG1	THR A	30	-1.428	66.186	51.107	1.00 50.68
	ATOM	227	CG2	THR A	30	-3.697	65.568	51.745	1.00 60.28
	ATOM	228	N	ARG A	31	-3,392	62.683	52.978	1.00 46.66
		229	CA						
	ATOM			ARG A	31	-4.404	61.987	53.734	1.00 47.88
5	ATOM	230	С	ARG A	31	-3.826	60.999	54.750	1.00 45.46
	ATOM	231	0	ARG A	31	-4.590	60.468	55.551	1.00 41.52
	ATOM	232	CB	ARG A	31	-5.335	61.214	52.805	1.00 56.73
	MOTA	233	CG	ARG A	31	-5.950	62.065	51.700	1.00 84.16
	ATOM	234	CD	ARG A	31	-7.338	61.568	51.284	1.00100.00
10									
10	MOTA	235	NE	ARG A	31	-7.344	60.450	50.327	1.00100.00
	MOTA	236	CZ	ARG A	31	-8.148	60.371	49.251	1.00100.00
	MOTA	237		ARG A	31	-9.034	61.324	48.944	1.00100.00
	MOTA	238	NH2	ARG A	31	-8.062	59.298	48.460	1.00100.00
	ATOM	239	N	ARG A	32	-2.489	60.752	54.683	1.00 39.71
15	ATOM	240	CA	ARG A	32	-1.751	59.798	55.531	1.00 39.09
	ATOM	241	C	ARG A	32	-2.324	58.411	55.379	
									1.00 39.62
	MOTA	242	0	ARG A	32	-2.495	57.655	56.337	1.00 33.10
	ATOM	243	CB	ARG A	32	-1.523	60.115	57.022	1.00 37.14
P	ATOM	244	CG	ARG A	32	-1.197	61.569	57.337	1.00 71.25
20	ATOM	245	CD	ARG A	32	0.277	61.834	57.686	1.00100.00
14.00	ATOM	246	NE	ARG A	32	0.703	61.299	58.986	1.00100.00
il.	ATOM		CZ						
les.		247		ARG A	32	1.284	62.005	59.961	1.00 79.51
# 3##>	ATOM	248		ARG A	32	1.522	63.308	59.831	1.00 55.73
## #[#0	ATOM	249	NH2	ARG A	32	1.626	61.387	61.098	1.00 44.96
25	ATOM	250	N	THR A	33	-2.612	58.068	54.139	1.00 39.83
LT	ATOM	251	CA	THR A	33	-3.162	56.752	53.902	1.00 39.31
	ATOM	252	С	THR A	33	-2.543	56.010	52.760	1.00 41.13
het.		253	Ö	THR A					
B .	ATOM				33	-1.853	56.574	51.926	1.00 42.93
lek-an	MOTA	254	CB	THR A	33	-4.635	56.835	53.641	1.00 43.44
30	MOTA	255	OG1	THR A	33	-4.798	57.636	52.468	1.00 40.17
n.	MOTA	256	CG2	THR A	33	-5.245	57.468	54.880	1.00 38.71
	MOTA	257	N	LEU A	34	-2.822	54.717	52.762	1.00 35.26
	ATOM	258	CA	LEU A	34	-2.372	53.799	51.745	1.00 35.20
1545 MIL.	ATOM	259	c	LEU A	34	-3.632	53.293	51.098	
35		260							1.00 32.49
	ATOM		0	LEU A	34	-4.474	52.670	51.751	1.00 30.96
	ATOM	261	CB	LEU A	34	-1.522	52.651	52.322	1.00 37.07
	ATOM	262	CG	LEU A	34	-0.149	52.571	51.685	1.00 42.99
	MOTA	263	CD1	LEU A	34	0.648	51.425	52.285	1.00 40.58
	ATOM	264	CD2	LEU A	34	-0.360	52.302	50.208	1.00 50.83
40	ATOM	265	N	THR A	35	-3.800	53.632	49.838	1.00 28.72
4 7	ATOM	266	CA	THR A	35	-5.017	53.228	49.198	1.00 31.26
	ATOM	267	C	THR A	35	-4.838	52.329	48.013	
									1.00 36.54
	ATOM	268	0	THR A	35	-3.940	52.546	47.187	1.00 34.70
	ATOM	269	CB	THR A	35	-5.877	54.427	48.813	1.00 44.88
45	MOTA	270	OG1		35	-5.484	55.549	49.579	1.00 58.59
	MOTA	271	CG2	THR A	35	-7.324	54.094	49.109	1.00 49.42
	MOTA	272	N	GLY A	36	-5.726	51.329	47.950	1.00 32.57
	ATOM	273	CA	GLY A	36	-5.696	50.405	46.837	1.00 33.89
	MOTA	274	c	GLY A	36	-6.418	49.074	46.993	1.00 34.50
50									
30	ATOM	275	0	GLY A	36	-7.441	48.919	47.678	1.00 31.78
	ATOM	276	N	THR A	37	-5.836	48.103	46.293	1.00 35.93
	ATOM	277	CA	THR A	37	-6.327	46.723	46.281	1.00 36.12
	ATOM	278	С	THR A	37	-5.268	45.696	46.473	1.00 35.67
	ATOM	279	0	THR A	37	-4.155	45.795	45.964	1.00 33.86
55	ATOM	280	CB	THR A	37	-7.119	46.306	45.050	1.00 42.21
	ATOM	281		THR A	37	-6.507			
1.0							46.804	43.870	1.00 30.98
	ATOM	282		THR A	37	-8.547	46.793	45.229	1.00 50.03
	ATOM	283	N	ALA A	38	-5.687	44.705	47.220	1.00 32.95
-	ATOM	284	CA	ALA A	38	-4.886	43.570	47.533	1.00 33.45
60	ATOM	285	С	ALA A	38	-5.481	42.374	46.824	1.00 35.47
	ATOM	286	0	ALA A	38	-6.580	41.906	47.151	1.00 32.91
	ATOM	287	CB	ALA A	38	-4.845	43.341	49.044	1.00 32.31
	MOTA	288	N	ALA A	39	-4.764			
							41.874	45.834	1.00 32.70
	MOTA	289	CA	ALA A	39	-5.274	40.702	45.140	1.00 31.59

	7001	200	~	777 7	20	4 600	20 464	45 770	1 00 00 11
	MOTA	290	C	ALA A	39	-4.692	39.464	45.770	1.00 32.11
	ATOM	291	0	ALA A	39	-3.514	39.147	45.608	1.00 32.46
	ATOM	292	CB	ALA A	39	-4.934	40.729	43.662	1.00 32.13
5	ATOM	293	N	LEU A	40	-5.505	38.774	46.508	1.00 27.06
3	ATOM	294	CA	LEU A	40	-5.001	37.593	47.155	1.00 29.04
	ATOM	295	C	LEU A	40	-5.331	36.322	46.364	1.00 36.88
	MOTA	296	0	LEU A	40	-6.485	36.100	45.963	1.00 28.89
	ATOM	297	CB	LEU A	40	-5.587	37.451	48.600	1.00 29.39
10	ATOM	298	CG	LEU A	40	-5.303	38.598	49.559	1.00 31.39
10	ATOM	299	CD1		40	-5.435	38.063	50.970	1.00 32.62
	ATOM	300	CD2		40	-3.879	39.019	49.355	1.00 31.60
	ATOM	301	N	THR A	41	-4.310	35.470	46.165	1.00 42.40
	ATOM	302	CA	THR A	41	-4.523	34.210	45.488	1.00 43.93
1.5	MOTA	303	С	THR A	41	-4.548	33.155	46.552	1.00 43.75
15	MOTA	304	0	THR A	41	-3.510	32.827	47.115	1.00 45.22
	ATOM	305	CB	THR A	41	-3.511	33.892	44.402	1.00 55.44
	MOTA	306	OG1		41	-3.604	34.885	43.418	1.00 55.57
	ATOM	307	CG2		41	-3.872	32.544	43.802	1.00 47.78
20	MOTA	308	N	VAL A	42	-5.755	32.688	46.848	1.00 33.25
20	ATOM	309	CA	VAL A	42	-5.946	31.720	47.893	1.00 32.21
I.	MOTA	310	С	VAL A	42	-6.166	30.312	47.380	1.00 40.56
	MOTA	311	0	VAL A	42	-6.827	30.105	46.376	1.00 42.56
	MOTA	312	CB	VAL A	42	-7.017	32.153	48.920	1.00 36.45
1FR 10 F	ATOM	313	CG1		42	-6.817	31.451	50.266	1.00 36.89
25	ATOM	314	CG2		42	-6.963	33.665	49.170	1.00 36.10
1	MOTA	315	N	GLN A	43	-5.590	29.357	48.117	1.00 35.91
}=4 ₄	ATOM	316	CA	GLN A	43	-5.678	27.945	47.838	1.00 31.59
202	MOTA	317	С	GLN A	43	-6.346	27.244	48.988	1.00 38.98
	MOTA	318	0	GLN A	43	-5.916	27.317	50.144	1.00 40.92
30	ATOM	319	CB	GLN A	43	-4.305	27.319	47.568	1.00 30.50
	ATOM	320	CG	GLN A	43	-4.362	25.800	47.259	1.00 53.80
T.)	ATOM	321	CD	GLN A	43	-2.986	25.177	47.099	1.00 62.47
in mil	MOTA	322	OE1		43	-2.569	24.842	45.978	1.00 57.34
35	ATOM	323	NE2		43	-2.274	25.037	48.224	1.00 43.72
35	MOTA	324	N	SER A	44	-7.423	26.555	48.664	1.00 33.83
*	MOTA	325	CA	SER A	44	-8.166	25.839	49.678	1.00 31.38
	ATOM	326	С	SER A	44	-7.495	24.557	50.117	1.00 42.10
	ATOM	327	0	SER A	44	-6.955	23.814	49.292	1.00 42.78
40	ATOM	328	CB	SER A	44	-9.576	25.530	49.226	1.00 28.60
40	ATOM	329	OG	SER A	44	-10.234	24.785	50.224	1.00 34.57
	ATOM	330	N	GLN A	45	-7.579	24.286	51.423	1.00 38.84
	MOTA	331	CA	GLN A	45	-7.007	23.082	51.994	1.00 37.05
	MOTA	332	С	GLN A	45	-8.082	22.050	52.269	1.00 47.57
1.5	ATOM	333	0	GLN A	45	-7.801	20.917	52.678	1.00 42.94
45	ATOM	334	CB	GLN A	45	-6.247	23.411	53.280	1.00 36.10
	MOTA	335	CG	GLN A	45	-5.246	24.539	53.034	1.00 54.73
	MOTA	336	CD	GLN A	45	-4.323	24.206	51.888	1.00 45.43
	MOTA	337	OE1		45	-4.257	24.888	50.833	1.00 39.23
50	MOTA	338		GLN A	45	-3.621	23.121	52.092	1.00 29.80
50	ATOM	339	N	GLU A	46	-9.330	22.459	52.048	1.00 50.54
	ATOM	340	CA	GLU A	46	-10.454	21.573	52.283	1.00 50.99
	ATOM	341	C	GLU A	46	-11.496	21.583	51.179	1.00 54.49
	MOTA	342	0	GLU A	46	-11.518	22.406	50.261	1.00 54.00
22	ATOM	343	CB	GLU A	46	-11.139	21.793	53.657	1.00 51.61
55	ATOM	344	CG	GLU A	46	-10.581	22.979	54.454	1.00 55.93
	MOTA	345	CD	GLU A	46	-11.427	23.329	55.646	1.00 78.67
	MOTA	346		GLU A	46	-12.563	23.765	55.543	1.00 69.56
	ATOM	347		GLU A	46	-10.814	23.129	56.796	1.00 75.10
20	ATOM	348	N	ASP A	47	-12.387	20.630	51.300	1.00 48.90
60	ATOM	349	CA	ASP A	47	-13.450	20.549	50.362	1.00 49.03
	ATOM	350	С	ASP A	47	-14.591	21.425	50.846	1.00 55.15
	ATOM	351	0	ASP A	47	-14.760	21.631	52.044	1.00 56.66
	MOTA	352	CB	ASP A	47	-13.913	19.099	50.227	1.00 50.20
	MOTA	353	CG	ASP A	47	-13.083	18.376	49.218	1.00 66.88

	ATOM	354		ASP A	47		12.340	18.945	48.434	1.00 66.27
	MOTA	355		ASP A	47		13.235	17.081	49.284	1.00 76.37
	ATOM	356 357	n ca	ASN A ASN A	48 48		15.391 16.519	21.941 22.755	49.929 50.339	1.00 50.25 1.00 48.45
5	ATOM ATOM	358	C	ASN A	48		16.115	24.000	51.115	1.00 43.43
,	ATOM	359	o	ASN A	48		16.699	24.351	52.138	1.00 39.78
	ATOM	360	CB	ASN A	48		17.559	21.909	51.117	1.00 51.19
	ATOM	361	CG	ASN A	48		18.985	22.417	51.005	1.00 76.39
	ATOM	362	OD1	ASN A	48		19.594	22.348	49.929	1.00 85.15
10	ATOM	363	ND2	ASN A	48	-	19.515	22.928	52.115	1.00 68.29
	MOTA	364	N	LEU A	49		15.113	24.688	50.628	1.00 35.36
	MOTA	365	CA	LEU A	49		14.728	25.874	51.335	1.00 34.40
	MOTA	366	С	LEU A	49		15.601	27.009	50.851	1.00 47.38
1.5	MOTA	367	0	LEU A	49		15.421	27.515	49.734	1.00 45.47
15	MOTA	368	CB	LEU A	49		13.239	26.152	51.173	1.00 31.04
	ATOM	369	CG	LEU A	49		12.781	27.394	51.885	1.00 29.82
	MOTA	370		LEU A	49		12.725	27.137 27.753	53.385	1.00 28.15
	ATOM ATOM	371 372	N N	ARG A	49 50		16.568	27.753	51.368 51.699	1.00 30.24 1.00 50.49
20	ATOM	373	CA	ARG A	50		17.560	28.392	51.401	1.00 50.49
42	ATOM	374	C	ARG A	50		17.169	29.838	51.702	1.00 55.57
W.	ATOM	375	Õ	ARG A	50		17.627	30.760	51.011	1.00 53.89
 - &	ATOM	376	CB	ARG A	50		18.928	28.028	51.986	1.00 58.35
" !**	ATOM	377	CG	ARG A	50		19.863	27.354	50.980	1.00 74.76
25	ATOM	378	CD	ARG A	50		20.438	26.024	51.462	1.00 81.60
अस्तु सर्	ATOM	379	NE	ARG A	50	-	21.214	25.355	50.415	1.00 94.37
UN.	ATOM	380	CZ	ARG A	50	-	22.465	24.888	50.538	1.00100.00
\$=# _k	ATOM	381	NH1	ARG A	50	-	23.151	24.990	51.687	1.00100.00
拳. ·	MOTA	382		ARG A	50		23.046	24.297	49.471	1.00 74.34
30	MOTA	383	N	SER A	51		16.331	30.006	52.743	1.00 54.71
T.	ATOM	384	CA	SER A	51		15.823	31.297	53.224	1.00 53.49
T.	ATOM	385	C	SER A	51		14.495	31.156	53.955	1.00 53.57
in the	MOTA	386 387	O	SER A	51 51		14.146	30.062	54.420	1.00 52.93
35	ATOM ATOM	388	CB OG	SER A	51		-16.788 -16.871	31.900 31.048	54.232 55.373	1.00 54.03 1.00 45.15
juk.	ATOM	389	N	LEU A	52		-13.796	32.298	54.067	1.00 45.15
	ATOM	390	CA	LEU A	52		-12.519	32.422	54.762	1.00 47.13
	ATOM	391	C	LEU A	52		12.415	33.671	55.640	1.00 50.43
	ATOM	392	0	LEU A	52		-13.145	34.633	55.471	1.00 52.64
40	ATOM	393	CB	LEU A	52		-11.235	32.117	53.923	1.00 44.20
	ATOM	394	CG	LEU A	52		-10.896	33.044	52.745	1.00 43.98
	ATOM	395		LEU A	52	-	-11.739	32.687	51.554	1.00 42.82
	ATOM	396		LEU A	52		-11.128	34.501	53.094	1.00 44.71
40	ATOM	397	N	VAL A	53		-11.483	33.658	56.579	1.00 44.97
45	ATOM	398	CA	VAL A	53	-	-11.271	34.781	57.455	1.00 41.69
	MOTA	399	C	VAL A	53		-9.859	35.309	57.339	1.00 44.25
	MOTA MOTA	400 401	O CB	VAL A VAL A	53 53	_	-8.866 -11.565	34.551 34.420	57.302	1.00 45.42 1.00 45.48
	ATOM	402		VAL A	53		-11.223	35.554	58.906 59.853	1.00 43.46
50	MOTA	403		VAL A	53		-13.030	34.073	59.050	1.00 45.79
	MOTA	404	N	LEU A	54		-9.796	36.627	57.166	1.00 45.75
	MOTA	405	CA	LEU A	54		-8.555	37.333	57.080	1.00 34.14
	ATOM	406	С	LEU A	54		-8.377	38.207	58.326	1.00 38.92
	ATOM	407	0	LEU A	54		-9.281	38.457	59.108	1.00 37.45
55	ATOM	408	CB	LEU A	54		-8.461	38.216	55.831	1.00 34.73
	ATOM	409	CG	LEU A	54		-8.539	37.469	54.510	1.00 40.25
	ATOM	410		LEU A	54		-8.416	38.488	53.374	1.00 40.69
	ATOM	411		LEU A	54		-7.424	36 .4 28	54.415	1.00 39.64
	MOTA	412	N	ASP A	55		-7.192	38.674	58.524	1.00 35.02
60	ATOM	413	CA	ASP A	55		-6.918	39.526	59.627	1.00 31.65
	ATOM	414	C	ASP A	55		-6.956	40.941	59.078	1.00 40.38
	ATOM	415	O	ASP A	55		-6.754	41.151	57.886	1.00 39.98
	ATOM	416	CB		55		-5.494	39.232	60.075	1.00 30.92
	ATOM	417	CG	ASP A	55		-5.397	38.103	61.037	1.00 35.96

	ATOM	418	OD1	ASP A	55	-6.049	38.074	62.066	1.00 38.49
	ATOM	419	OD2	ASP A	55	-4.491	37.205	60.682	1.00 36.53
	ATOM	420	N	THR A	56	-7.196	41.900	59.963	1.00 42.93
	ATOM	421	CA	THR A	56	-7.243	43.334	59.661	1.00 41.75
5	ATOM	422	С	THR A	56	-7.101	44.128	60.967	1.00 37.46
	MOTA	423	0	THR A	56	-7.517	43.687	62.049	1.00 36.98
	ATOM	424	CB	THR A	56	-8.514	43.825	58.894	1.00 37.17
· ·	ATOM	425	OG1	THR A	56	-9.587	43.957	59.805	1.00 31.84
	ATOM	426	CG2	THR A	56	-8.910	42.943	57.714	1.00 33.58
10	ATOM	427	N	LYS A	57	-6.513	45.304	60.863	1.00 26.63
	MOTA	428	CA	LYS A	57	-6.363	46.134	62.020	1.00 25.64
	MOTA	429	С	LYS A	57	-6.585	47.539	61.547	1.00 30.08
	MOTA	430	0	LYS A	57	-5.854	48.012	60.711	1.00 25.68
	MOTA	431	CB	LYS A	57	-4.991	45.983	62.641	1.00 27.34
15	MOTA	432	CG	LYS A	57	-4.907	46.387	64.100	1.00 35.83
	ATOM	433	CD	LYS A	57	-3.514	46.904	64.471	1.00 35.57
	ATOM	434	CE	LYS A	57	-2.901	46.225	65.689	1.00 50.54
	MOTA	435	NZ	LYS A	57	-2.521	47.180	66.757	1.00 55.43
20	ATOM	436	N	ASP A	58	-7.617	48.188	62.065	1.00 32.68
20	ATOM	437	CA	ASP A	58	-7.895	49.545	61.665	1.00 35.27
185±21 , 1970.	ATOM	438	C	ASP A	58	-7.894	49.710	60.149	1.00 38.24
	ATOM	439	0	ASP A	58	-7.289	50.627	59.571	1.00 35.86
į.	ATOM	440	CB	ASP A	58	-6.968	50.550	62.386	1.00 37.22
25	ATOM	441	CG	ASP A	58	-7.041	50.393	63.880	1.00 50.71
25	ATOM	442		ASP A	58	-8.073	50.136	64.478	1.00 57.20
LT	ATOM	443		ASP A	58	-5.878	50.562	64.463	1.00 45.82
J-4.	ATOM	444	N	LEU A	59	-8.604	48.796	59.516	1.00 37.68
	ATOM	445	CA	LEU A	59	-8.720	48.813	58.079	1.00 39.36
30	ATOM	446	С 0	LEU A	59 59	-10.077	49.243	57.555	1.00 45.51
	ATOM ATOM	447 448	СВ	LEU A	59	-11.146 -8.265	48.946 47.506	58.120 57.422	1.00 44.18
	ATOM	449	CG	LEU A	59	-6.762	47.475	57.422	1.00 38.42 1.00 37.40
	ATOM	450	CD1		59	-6.392	46.173	56.526	1.00 37.40
1 T	ATOM	451		LEU A	59	-6.321	48.655	56.361	1.00 36.57
35	ATOM	452	N	THR A	60	-9.984	49.949	56.437	1.00 30.57
j-A.	ATOM	453	CA	THR A	60	-11.132	50.483	55.734	1.00 42.63
	ATOM	454	c	THR A	60	-11.357	49.705	54.463	1.00 38.18
	ATOM	455	ō	THR A	60	-10.632	49.856	53.454	1.00 34.33
	ATOM	456	CB	THR A	60	-11.030	52.028	55.532	1.00 65.15
40	ATOM	457	OG1		60	-11.806	52.736	56.504	1.00 67.56
	ATOM	458	CG2	THR A	60	-11.345	52.480	54.104	1.00 56.89
	ATOM	459	N	ILE A	61	-12.360	48.847	54.571	1.00 33.39
	ATOM	460	CA	ILE A	61	-12.753	47.975	53.482	1.00 35.89
	ATOM	461	С	ILE A	61	-13.726	48.634	52.533	1.00 41.05
45	ATOM	462	0	ILE A	61	-14.913	48.706	52.840	1.00 40.08
	ATOM	463	CB	ILE A	61	-13.403	46.670	53.944	1.00 39.71
	ATOM	464	CG1	ILE A	61	-12.482	45.826	54.832	1.00 39.90
	MOTA	465	CG2	ILE A	61	-13.788	45.900	52.691	1.00 38.96
	ATOM	466	CD1	ILE A	61	-11.027	45.851	54.358	1.00 49.61
50	MOTA	467	N	GLU A	62	-13.219	49.080	51.391	1.00 40.23
	ATOM	468	CA	GLU A	62	-14.040	49.700	50.365	1.00 41.73
	ATOM	469	С	GLU A	62	-14.986	48.633	49.826	1.00 47.09
	MOTA	470	0	GLU A	62	-16.207	48.726	49.926	1.00 47.52
	MOTA	471	CB	GLU A	62	-13.138	50.272	49.239	1.00 44.08
55	ATOM	472	CG	GLU A	62	-13.765	51.406	48.381	1.00 64.08
	MOTA	473	CD	GLU A	62	-14.686	50.946	47.256	1.00100.00
	ATOM	474		GLU A	62	-15.458	50.002	47.376	1.00100.00
	ATOM	475		GLU A	62	-14.591	51.670	46.146	1.00 75.11
C 0	ATOM	476	N	LYS A	63	-14.399	47.580	49.267	1.00 43.46
60	ATOM	477	CA	LYS A	63	-15.168	46.474	48.746	1.00 40.53
	ATOM	478	С	LYS A	63	-14.250	45.307	48.489	1.00 45.38
	ATOM	47.9	0	LYS A	63	-13.046	45.500	48.362	1.00 43.51
	ATOM	480	CB	LYS A	63	-15.818	46.830	47.428	1.00 40.46
	ATOM	481	CG	LYS A	63	-14.789	46.959	46.321	1.00 20.53

	MOTA	482	CD	LYS A	63	-15.367	47.555	45.054	1.00 28.36
	ATOM	483	CE	LYS A	63	-14.315	48.158	44.139	1.00 40.61
	MOTA	484	NZ	LYS A	63	-14.588	47.938	42.711	1.00 54.71
_	MOTA	485	N	VAL A	64	-14.862	44.116	48.441	1.00 45.57
5	ATOM	486	CA	VAL A	64	-14.190	42.844	48.171	1.00 44.90
	MOTA	487	С	VAL A	64	-14.666	42.263	46.841	1.00 46.44
	ATOM	488	0	VAL A	64	-15.826	41.917	46.700	1.00 45.81
	ATOM	489	CB	VAL A	64	-14.505	41.748	49.192	1.00 46.24
	ATOM	490	CG1	VAL A	64	-13.864	40.471	48.669	1.00 44.81
10				VAL A					
10	ATOM	491			64	-14.040	42.048	50.627	1.00 44.77
	MOTA	492	N	VAL A	65	-13.793	42.099	45.875	1.00 43.10
	ATOM	493	CA	VAL A	65	-14.240	41.537	44.604	1.00 41.42
	ATOM	494	С	VAL A	65	-13.707	40.156	44.282	1.00 42.13
4.5	MOTA	495	0	VAL A	65	-12.605	39.787	44.660	1.00 42.64
15	ATOM	496	CB	VAL A	65	-13.856	42.462	43.484	1.00 44.58
	ATOM	497	CG1	VAL A	65	-14.520	42.037	42.189	1.00 42.79
	ATOM	498		VAL A	65	-14.264	43.874	43.883	
									1.00 45.05
	ATOM	499	N	ILE A	66	-14.515	39.402	43.556	1.00 38.68
and AB	MOTA	500	CA	ILE A	66	-14.179	38.053	43.113	1.00 39.98
20	MOTA	501	С	ILE A	66	-14.899	37.774	41.802	1.00 44.86
41									
125 (EF) 1 20),	MOTA	502	0	ILE A	66	-16.136	37.735	41.729	1.00 42.69
	MOTA	503	CB	ILE A	66	-14.520	36.947	44.113	1.00 44.28
la.	ATOM	504	CG1	ILE A	66	-13.813	37.127	45.445	1.00 47.27
a 1002.		505		ILE A	66				
······································	ATOM					-14.141	35.578	43.550	1.00 42.84
25	MOTA	506	CDI	ILE A	66	-14.352	36.169	46.514	1.00 38.79
14 E ****	ATOM	507	N	ASN A	67	-14.120	37.549	40.759	1.00 42.94
U1	ATOM	508	CA	ASN A	67	-14.715	37.266	39.472	1.00 44.24
#	MOTA	509	С	ASN A	67	-15.541	38.444	39.008	1.00 54.25
果	MOTA	510	0	ASN A	67	-16.743	38.344	38.768	1.00 57.56
30	MOTA	511	CB	ASN A	67	-15.595	36.007	39.507	1.00 40.72
	ATOM	512	CG	ASN A	67	-14.788	34.759	39.745	
T.									1.00 57.39
	ATOM	513		ASN A	67	-13.581	34.711	39.454	1.00 52.63
100 45°	ATOM	514	ND2	ASN A	67	-15.446	33.760	40.317	1.00 44.54
77 F	ATOM	515	N	GLY A	68	-14.876	39.574	38.899	1.00 50.43
35									
	ATOM	516	CA	GLY A	68	-15.517	40.796	38.462	1.00 48.89
 - -	ATOM	517	С	GLY A	68	-16.807	41.115	39.194	1.00 48.77
	ATOM	518	0	GLY A	68	-17.523	42.018	38.803	1.00 51.39
	ATOM	519	N	GLN A	69	-17.129	40.385	40.244	1.00 40.06
40	ATOM	520	CA	GLN A	69	-18.348	40.716	40.928	1.00 40.02
40	ATOM	521	С	GLN A	69	-18.031	41.059	42.364	1.00 50.45
	ATOM	522	0	GLN A	69	-16.943	40.748	42.855	1.00 50.53
	ATOM	523	CB	GLN A	69	-19.415	39.602	40.829	1.00 40.78
	ATOM	524	CG	GLN A	69	-19.966	39.367	39.414	1.00 23.77
	ATOM	525	CD	GLN A	69	-20.513	40.646	38.831	1.00 56.53
45	ATOM	526	OE1	GLN A	69	-19.974	41.198	37.859	1.00 55.28
	MOTA	527		GLN A	69	-21.588	41.134		
								39.437	1.00 62.26
	ATOM	528	N	GLU A	70	-18.975	41.718	43.028	1.00 49.43
	ATOM	529	CA	GLU A	70	-18.766	42.094	44.407	1.00 50.67
	ATOM	530	С	GLU A	70	-19.296	40.996	45.288	1.00 57.90
50	ATOM	531	0	GLU A	70	-20.272	40.367	44.909	1.00 63.90
50									
	ATOM	532	CB	GLU A	70	-19.449	43.434	44.732	1.00 52.26
	MOTA	533	CG	GLU A	70	-18.824	44.624	43.970	1.00 64.80
	ATOM	534	CD	GLU A	70	-19.181	45.967	44.555	1.00 91.82
	ATOM	535		GLU A	70	-19.749	46.108	45.629	
55									1.00100.00
در	ATOM	536		GLU A	70	-18.814	46.963	43.785	1.00 76.01
	ATOM	537	N	VAL A	71	-18.655	40.742	46.433	1.00 47.28
	ATOM	538	CA	VAL A	71	-19.119	39.685	47.335	1.00 43.84
	ATOM	539	C	VAL A					
					71	-19.434	40.153	48.768	1.00 41.62
~ ^	MOTA	540	0	VAL A	71	-18.983	41.206	49.254	1.00 35.70
60	MOTA	541	CB	VAL A	71	-18.308	38.361	47.273	1.00 46.05
	ATOM	542		VAL A	71	-18.062	37.923	45.827	1.00 45.19
	ATOM	543		VAL A	71	-16.979	38.460	48.017	1.00 45.24
	ATOM	544	N	LYS A	72	-20.239	39.343	49.431	1.00 39.34
	ATOM	545	CA	LYS A	72	-20.610	39.594	50.792	1.00 42.40

	MOTA	546	С	LYS A	72		39.466	51.668	1.00 56.92
	MOTA	547	0	LYS A	72	-18.399	38.729	51.334	1.00 59.27
	ATOM	548	CB	LYS A	72	-21.719	88.629	51.211	1.00 45.76
	ATOM	549	CG	LYS A	72		88.960	52.557	1.00 86.98
_									
5	ATOM	550	CD	LYS A	72		38.767	52.606	1.00100.00
	ATOM	551	CE	LYS A	72	-24.656	10.012	53.077	1.00100.00
	ATOM	552	NZ	LYS A	72	-26.011 3	39.730	53.592	1.00100.00
	ATOM	553	N	TYR A	73	-19.332	10.210	52.780	1.00 55.45
	ATOM	554	CA	TYR A	73		10.226	53.747	1.00 53.31
10									
10	MOTA	555	C	TYR A	73		10.884	55.068	1.00 50.87
	MOTA	556	0	TYR A	73		11.703	55.139	1.00 47.82
	MOTA	557	CB	TYR A	73	-16.891	10.741	53.214	1.00 52.73
	MOTA	558	CG	TYR A	73	-16.765	12.244	53.227	1.00 51.76
	MOTA	559	CD1	TYR A	73		12.946	54.416	1.00 52.82
15	ATOM	560		TYR A	73		12.967	52.039	1.00 53.30
1.5									
	ATOM	561	CE1		73		44.340	54.422	1.00 52.71
	ATOM	562	CE2	TYR A	73		44.359	52.026	1.00 55.39
	ATOM	563	CZ	TYR A	73	-16.592	45.044	53.229	1.00 63.45
	ATOM	564	OH	TYR A	73	-16.471	46.404	53.215	1.00 69.53
1 20	ATOM	565	N	ALA A	74		40.494	56.112	1.00 45.37
							10.999		
42	ATOM	566	CA	ALA A	74			57.433	1.00 42.62
riji.	MOTA	567	С	ALA A	74		41.265	58.222	1.00 47.81
ļ ∌ ķ ,	ATOM	568	O-	ALA A	74	-15.894	40.554	58.133	1.00 45.50
	ATOM	569	CB	ALA A	74	-19.111	40.035	58.170	1.00 40.75
25	ATOM	570	N	LEU A	75	-16.930	42.323	59.005	1.00 49.02
4570	ATOM	571	CA	LEU A	75		42.693	59.869	1.00 48.85
Ú1									
## W	MOTA	572	C	LEU A	75		42.464	61.281	1.00 47.18
je Iv	MOTA	573	0	LEU A	75		43.021	61.687	1.00 44.35
**	ATOM	574	CB	LEU A	75	-15.332	44.136	59.675	1.00 49.64
30	ATOM	575	CG	LEU A	75	-14.789	44.357	58.270	1.00 58.09
# The second	MOTA	576	CD1	LEU A	75	-14.524	45.841	58.023	1.00 61.34
ñ.	MOTA	577		LEU A	75		43.565	58.069	1.00 62.34
T.									
12 1	MOTA	578	N	GLY A	76		41.592	62.004	1.00 47.67
Sarati	MOTA	579	CA	GLY A	76		41.281	63.359	1.00 46.79
35	MOTA	580	С	GLY A	76	-15.495	42.337	64.279	1.00 47.74
l+ 4.	ATOM	581	0	GLY A	76	-14.656	43.171	63.882	1.00 42.87
	ATOM	582	N	GLU A	77	-15.988	42.311	65.502	1.00 48.32
	ATOM	583	CA	GLU A	77		43.300	66.431	1.00 52.14
	ATOM	584	C	GLU A	77		43.195	66.679	1.00 56.71
40									
40	ATOM	585	0	GLU A	77		42.120	66.591	1.00 55.78
	ATOM	586	CB	GLU A	77		43.341	67.732	1.00 55.55
	ATOM	587	CG	GLU A	77	-17.198	42.063	67.969	1.00 79.57
	ATOM	588	CD	GLU A	77	-17.440	41.739	69.427	1.00100.00
	ATOM	589	OE1	GLU A	77		41.435	70.211	1.00100.00
45	ATOM	590		GLU A	77		41.799	69.770	1.00100.00
••		591	N	ARG A	78		44.344	67.000	1.00 54.17
	MOTA								
	ATOM	592	CA	ARG A	78		44.433	67.298	1.00 53.38
	MOTA	593	С	ARG A	78		43.656	68.579	1.00 58.88
	ATOM	594	0	ARG A	78	-12.247	43.767	69.635	1.00 61.35
50	MOTA	595	CB	ARG A	78	-11.571	45.891	67.367	1.00 41.96
	MOTA	596	CG	ARG A	78		46.006	67.326	1.00 38.20
	MOTA	597	CD	ARG A	78		47.411	67.551	1.00 44.73
	ATOM	598	NE	ARG A	78		47.648	66.842	1.00 66.47
بر سر	MOTA	599	CZ	ARG A	78		48.247	67.389	1.00 97.61
55	MOTA	600		ARG A	78		48.692	68.645	1.00100.00
	ATOM	601	NH2	ARG A	78	-6.151	48.413	66.663	1.00 80.10
	ATOM	602	N	GLN A	79		42.857	68.463	1.00 49.54
	ATOM	603	CA	GLN A	79		42.115	69.566	1.00 47.71
			C	GLN A	79				
<i>Δ</i> Λ	ATOM	604					42.789	69.865	1.00 49.77
60	ATOM	605	0	GLN A	79		42.421	69.333	1.00 52.63
	ATOM	606	CB	GLN A	79		40.613	69.240	1.00 49.05
	ATOM	607	CG	GLN A	79	-11.109	39.794	69.339	1.00 57.32
	ATOM	608	CD	GLN A	79		38.435	68.656	1.00 69.51
	ATOM	609		GLN A	79		37.480	69.152	1.00 49.72
		300							

	ATOM	610	NE2	GLN A	79		-11.727	38.340	67.517	1.00 62.60
	ATOM	611	N	SER A	80					
							-8.699	43.826	70.683	1.00 41.74
	ATOM	612	CA	SER A	80		-7.490	44.543	71.022	1.00 37.90
_	ATOM	613	С	SER A	80		-6.437	44.559	69.920	1.00 35.98
5	ATOM	614	0	SER A	80		-6.736	44.939	68.801	1.00 34.52
	ATOM	615	CB	SER A	80		-6.910	44.144	72.372	1.00 39.07
	ATOM	616	OG	SER A	80		-7.255		72.684	
		617	N			,		42.803		1.00 61.32
	ATOM			TYR A	81		-5.206	44.154	70.289	1.00 29.92
10	ATOM	618	CA	TYR A	81		-4.027	44.114	69.430	1.00 26.45
10	MOTA	619	С	TYR A	81		-4.163	43.116	68.285	1.00 30.82
	ATOM	620	0	TYR A	81		-3.480	43.215	67.269	1.00 34.48
	ATOM	621	СВ	TYR A	81		-2.727			
								43.893	70.257	1.00 25.19
	ATOM	622	CG	TYR A	81		-2.713	42.491	70.839	1.00 24.57
4.5	MOTA	623		TYR A	81		-3.327	42.247	72.066	1.00 27.27
15	MOTA	624	CD2	TYR A	81		-2.165	41.410	70.148	1.00 21.82
	ATOM	625	CE1	TYR A	81		-3.380	40.975	72.632	1.00 26.49
	ATOM	626		TYR A	81		-2.230	40.122		
	ATOM	627	CZ	TYR A					70.682	1.00 23.48
					81		-2.827	39.908	71.930	1.00 38.28
	MOTA	628	OH	TYR A	81		-2.889	38.653	72.493	1.00 42.17
20	MOTA	629	N	LYS A	82		-5.038	42.136	68.415	1.00 26.97
ul)	MOTA	630	CA	LYS A	82		-5.170	41.229	67.293	1.00 27.99
	ATOM	631	C	LYS A	82					
							-5.867	41.898	66.072	1.00 38.90
25	MOTA	632	0	LYS A	82		-5.614	41.541	64.900	1.00 37.15
F=0	MOTA	633	CB	LYS A	82		-5.785	39.918	67.708	1.00 27.59
25	ATOM	634	CG	LYS A	82		-5.169	39.451	69.008	1.00 39.68
	ATOM	635	CD	LYS A	82		-5.435	37.993	69.350	
J-A										1.00 46.78
Same.	ATOM	636	CE	LYS A	82		-6.414	37.819	70.492	1.00 59.84
38	ATOM	637	NZ	LYS A	82		-7.097	36.523	70.452	1.00 63.48
	MOTA	638	N	GLY A	83		-6.738	42.894	66.367	1.00 35.64
30	MOTA	639	CA	GLY A	83		-7.512	43.620	65.368	1.00 33.65
	ATOM	640	С	GLY A	83		-8.866	42.925	65.111	
	ATOM	641	ō	GLY A	83					1.00 32.95
12							-9.297	42.063	65.870	1.00 28.28
SERVICE SERVIC	ATOM	642	N	SER A	84		-9.535	43.300	64.026	1.00 34.51
35	ATOM	643	CA	SER A	84		-10.839	42.742	63.673	1.00 36.13
3 3	ATOM	644	С	SER A	84		-10.796	41.724	62.549	1.00 40.65
off and a	ATOM	645	0	SER A	84		-10.173	41.893	61.501	1.00 39.77
	ATOM	646	СВ	SER A	84		-11.883	43.808		
	ATOM	647	OG						63.383	1.00 37.68
				SER A	84		-11.812	44.832	64.352	1.00 45.14
40	ATOM	648	N	PRO A	85		-11.491	40.656	62.791	1.00 37.01
40	ATOM	649	CA	PRO A	85		-11.573	39.559	61.863	1.00 34.91
	ATOM	650	С	PRO A	85		-12.459	39.946	60.712	1.00 35.92
	ATOM	651	0	PRO A	85		-13.514	40.522	60.941	1.00 35.32
	MOTA	652	CB	PRO A	85					
							-12.227	38.406	62.647	1.00 37.00
AE	ATOM	653	CG	PRO A	85		-12.714	38.981	63.974	1.00 44.97
45	MOTA	654	CD	PRO A	85		-12.325	40.462	64.004	1.00 40.72
	ATOM	655	N	MET A	86		-12.018	39.642	59.487	1.00 30.47
	ATOM	656	CA	MET A	86		-12.756	39.960	58.275	1.00 28.55
	ATOM	657	С	MET A	86		-13.165			
	MOTA	658	Õ					38.683	57.552	1.00 40.49
50				MET A	86		-12.338	38.015	56.954	1.00 39.69
30	ATOM	659	CB	MET A	86		-11.921	40.829	57.337	1.00 29.51
	MOTA	660	CG	MET A	86		-12.750	41.242	56.136	1.00 37.40
	ATOM	661	SD	MET A	86		-11.816	41.878	54.701	1.00 47.84
	ATOM	662	CE	MET A	86		-13.244	42.527		
	ATOM	663	N						53.805	1.00 46.52
55				GLU A	87		-14.441	38.324	57.610	1.00 44.34
رر	ATOM	664	CA	GLU A	87		-14.912	37.107	56.950	1.00 47.21
	ATOM	665	С	GLU A	87		-15.495	37.352	55.560	1.00 51.53
	ATOM	666	0	GLU A	87		-16.425	38.129	55.424	1.00 53.92
	MOTA	667	CB	GLU A	87		-15.942			
	ATOM	668	CG	GLU A				36.390	57.813	1.00 49.46
60					87		-16.144	34.937	57.389	1.00 56.39
UU	ATOM	669	CD	GLU A	87		-17.300	34.316	58.104	1.00 80.78
	MOTA	670		GLU A	87		-18.439	34.738	57.994	1.00 86.69
	MOTA	671	OE2	GLU A	87		-16.943	33.301	58.868	1.00 68.69
	MOTA	672	N	ILE A	88		-14.942			
	ATOM	673	CA	ILE A				36.659	54.544	1.00 43.84
	AION	013	CA.	The W	88		-15.332	36.765	53.145	1.00 40.15

	ATOM	674	С	ILE A	88	-16.145	35.610	52.613	1.00 46.72
	ATOM	675	ō	ILE A	88	-15.725			
	ATOM	676	СВ	ILE A			34.460	52.656	1.00 48.10
					88	-14.107	36.891	52.292	1.00 39.13
-	ATOM	677		ILE A	88	-13.328	38.146	52.696	1.00 38.40
5	ATOM	678	CG2	ILE A	88	-14.538	36.932	50.839	1.00 28.13
	ATOM	679	CD1	ILE A	88	-11.944	38.200	52.051	1.00 30.07
	ATOM	680	N	SER A	89	-17.314	35.931	52.077	
	ATOM	681	CA	SER A					1.00 45.16
					89	-18.181	34.893	51.559	1.00 44.76
	ATOM	682	С	SER A	89	-17.902	34.531	50.131	1.00 46.01
10	ATOM	683	0	SER A	89	-18.048	35.347	49.243	1.00 44.34
	MOTA	684	CB	SER A	89	-19.657	35.121	51.827	1.00 51.87
	ATOM	685	OG	SER A	89	-19.942	34.834	53.198	1.00 69.07
	ATOM	686	N	LEU A	90	-17.494	33.279		
								49.914	1.00 46.43
1.5	ATOM	687	CA	LEU A	90	-17.204	32.804	48.575	1.00 46.93
15	MOTA	688	С	LEU A	90	-18.450	32.235	47.935	1.00 55.26
	ATOM	689	0	LEU A	90	-19.210	31.476	48.556	1.00 54.94
	ATOM	690	CB	LEU A	90	-16.080	31.750	48.521	1.00 46.14
alterior.	ATOM	691	CG	LEU A	90	-15.262	31.607	49.792	1.00 50.78
		692		LEU A					
20	ATOM				90	-14.546	30.261	49.806	1.00 50.27
- 2U	ATOM	693	CD2	LEU A	90	-14.219	32.708	49.863	1.00 55.52
41	MOTA	694	N	PRO A	91	-18.626	32.607	46.683	1.00 54.81
j.k.	ATOM	695	CA	PRO A	91	-19.756	32.183	45.870	1.00 58.45
ndaw Sast	ATOM	696	C	PRO A	91	-19.585	30.782	45.254	
. मुक्ता इसद	ATOM	697	Ö	PRO A	91				1.00 67.78
25						-20.500	30.250	44.623	1.00 68.64
25	ATOM	698	CB	PRO A	91	-19.843	33.213	44.738	1.00 59.70
j. L	MOTA	699	CG	PRO A	91	-18.503	33.952	44.711	1.00 61.25
	ATOM	700	CD	PRO A	91	-17.731	33.539	45.961	1.00 54.16
123	ATOM	701	N	ILE A	92	-18.413	30.177	45.416	1.00 64.82
j.a.	ATOM	702	CA	ILE A	92	-18.210	28.863		
30	ATOM	703						44.850	1.00 65.03
			С	ILE A	92	-17.485	27.948	45.801	1.00 66.34
T.	ATOM	704	0	ILE A	92	-16.258	27.984	45.865	1.00 70.20
	ATOM	705	CB	ILE A	92	-17.433	28.927	43.547	1.00 69.56
22 M	ATOM	706	CG1	ILE A	92	-18.298	29.495	42.430	1.00 70.02
	ATOM	707		ILE A	92	-16.975	27.517	43.171	1.00 71.86
1 35	MOTA	708		ILE A	92				
22						-17.528	29.672	41.121	1.00 80.63
	ATOM	709	N	ALA A	93	-18.219	27.115	46.534	1.00 54.40
	ATOM	710	CA	ALA A	93	-17.526	26.247	47.452	1.00 51.74
	MOTA	711	С	ALA A	93	-16.265	25.750	46.804	1.00 52.66
	ATOM	712	0	ALA A	93	-16.288	25.319	45.662	1.00 49.87
40	MOTA	713	CB	ALA A	93	-18.367	25.101	47.968	1.00 52.76
	ATOM	714	N	LEU A	94	-15.162			
	ATOM						25.861	47.544	1.00 48.18
		715	CA	LEU A	94	-13.862	25.425	47.067	1.00 43.27
	MOTA	716	С	LEU A	94	-13.566	24.066	47.581	1.00 43.98
	ATOM	717	0	LEU A	94	-14.086	23.633	48.601	1.00 44.63
45	ATOM	718	CB	LEU A	94	-12.713	26.344	47.509	1.00 41.05
	ATOM	719	CG	LEU A	94	-12.685	27.638	46.739	1.00 40.03
	ATOM	720		LEU A	94	-11.272			
	ATOM	721					28.200	46.751	1.00 36.88
				LEU A	94	-13.115	27.343	45.311	1.00 44.98
50	MOTA	722	N	SER A	95	-12.706	23.406	46.875	1.00 43.26
50	ATOM	723	CA	SER A	95	-12.321	22.074	47.256	1.00 43.76
	ATOM	724	C	SER A	95	-10.807	21.991	47.344	1.00 38.58
	ATOM	725	0	SER A	95	-10.087	22.944	46.975	
	ATOM	726	СВ	SER A	95	-12.902			1.00 36.78
	•						21.092	46.256	1.00 51.55
55	ATOM	727	OG	SER A	95	-14.299	21.305	46.156	1.00 62.74
	ATOM	728	N	LYS A	96	-10.321	20.863	47.830	1.00 31.10
	ATOM	729	CA	LYS A	96	-8.883	20.723	47.958	1.00 34.92
	ATOM	730	С	LYS A	96	-8.058	21.238	46.777	1.00 45.63
	ATOM	731	ŏ	LYS A	96	-8.400			
	ATOM	732	CB				21.063	45.612	1.00 49.35
60				LYS A	96	-8.401	19.366	48.451	1.00 38.53
oo	ATOM	733	CG	LYS A	96	-9.189	18.871	49.651	1.00 68.97
	ATOM	734	CD	LYS A	96	-8.691	17.549	50.221	1.00 80.86
	ATOM	735	CE	LYS A	96	-9.596	17.011	51.330	1.00 92.53
	ATOM	736	NZ	LYS A	96	-9.049	15.833	52.029	1.00100.00
	ATOM	737	N	ASN A	97	-6.944			
		,		- 10-11	٠,	0.944	21.873	47.108	1.00 41.92

	ATOM	738	CA	ASN A	97	-6.009	22.403	46.139	3 00	40.91
	ATOM	739	С	ASN A	97	-6.606	23.348	45.088		42.64
	ATOM	740	0	ASN A	97	-5.963	23.681	44.068		
	ATOM	741	CB	ASN A	97	-5.084	21.304			38.69
5	ATOM	742	CG	ASN A	97			45.583		28.16
-						-4.327	20.568	46.677		52.21
	ATOM	743		ASN A	97	-3.089	20.627	46.744		55.30
	ATOM	744		ASN A		-5.060	19.858	47.533	1.00	53.87
	ATOM	745	N	GLN A	98	-7.833	23.791	45.382	1.00	36.59
	ATOM	746	CA	GLN A	98	-8.557	24.718	44.536		38.44
10	ATOM	747	С	GLN A	98	-8.288	26.181	44.951		43.30
	ATOM	748	0	GLN A	98	-8.248	26.526	46.138		43.40
	ATOM	749	CB	GLN A	98	-10.064	24.395	44.575		42.26
	ATOM	750	CG	GLN A	98	-10.553	23.538	43.385		
	ATOM	751	CD	GLN A	98	-12.008	23.778			68.24
15	ATOM	752	OE1	GLN A	98			43.010		95.57
1.0		753				-12.890	22.935	43.278		86.92
	ATOM		NE2	GLN A	98	-12.271	24.935	42.393		95.48
	ATOM	754	N	GLU A	99	-8.089	27.062	43.973	1.00	39.70
24 m	ATOM	755	CA	GLU A	99	-7.817	28.468	44.280	1.00	40.49
120	ATOM	756	С	GLU A	99	-8.750	29.536	43.683		47.84
20	MOTA	757	0	GLU A	99	-9.330	29.394	42.606		46.85
	ATOM	758	CB	GLU A	99	-6.361	28.866	43.951		40.24
]=# ₄	ATOM	759	CG	GLU A	99	-5.608	27.861	43.080		44.16
indus:	ATOM	760	CD	GLU A	99	-4.120	28.119	42.990		
initial and initia	ATOM	761	OE1	GLU A	99	-3.636				65.64
25	ATOM	762	OE2	GLU A	99		29.062	42.376		73.95
¥ ¥23						-3.395	27.210	43.614		55.99
# # #.≽	ATOM	763	N	ILE A		-8.848	30.643	44.418		43.55
a	ATOM	764	CA	ILE A		-9.595	31.800	44.005	1.00	43.46
jas.	ATOM	765	С	ILE A		-8.701	32.992	44.238	1.00	53.31
	ATOM	766	0	ILE A		-7.725	32.927	45.004	1.00	55.16
30	ATOM	767	CB	ILE A	100	-10.881	32.068	44.773	1.00	46.65
	ATOM	768	CG1	ILE A	100	-10.762	31.640	46.227		50.76
### ###	ATOM	769	CG2	ILE A	100	-12.111	31.486	44.106		46.76
	ATOM	770	CD1	ILE A		-9.959	32.620	47.087		64.36
2.7	ATOM	771	N	VAL A		-9.060	34.076	43.580		48.20
35	ATOM	772	CA	VAL A		-8.382	35.329	43.760		
	ATOM	773	C	VAL A		-9.383				45.63
	ATOM	774	Ö	VAL A			36.351			48.59
	ATOM	775	СВ	VAL A		-10.331	36.722	43.623		51.29
						-7.461	35.793	42.633		45.06
40	ATOM	776	CG1	VAL A		-7.693	35.000	41.378		43.25
40	ATOM	777		VAL A		-7.609	37.289	42.395	1.00	45.02
	ATOM	778	N	ILE A		-9.182	36.738	45.546	1.00	41.15
	MOTA	779	CA	ILE A		-10.023	37.690	46.238	1.00	39.43
	ATOM	780	С	ILE A	102	-9.439	39.062	46.170	1.00	49.35
	ATOM	781	0	ILE A	102	-8.331	39.274	46.659		53.80
45	ATOM	782	CB	ILE A	102	-10.097	37.319	47.694		39.19
	ATOM	783	CG1	ILE A		-10.180	35.800	47.809		35.28
	ATOM	784	CG2	ILE A	102	-11.300	37.992	48.341		35.25
	ATOM	785	CD1	ILE A	102	-10.962	35.392	49.044		47.09
	ATOM	786	N	GLU A		-10.192	39.984			
50	ATOM	787	CA	GLU A		-9.748		45.572		43.20
	ATOM	788	C	GLU A			41.362	45.433		39.88
	ATOM	789				-10.378	42.299	46.425		44.03
			0	GLU A		-11.580	42.558	46.385		41.34
	ATOM	790	CB	GLU A		-9.950	41.930	44.047	1.00	39.11
EE	ATOM	791	CG	GLU A		-9.017	43.112	43.863	1.00	36.18
55	ATOM	792	CD	GLU A		-9.150	43.666	42.485	1.00	61.93
	ATOM	793	OE1	GLU A	103	-10.157	44.234	42.100		69.89
	ATOM	794	OE2	GLU A	103	-8.087	43.457	41.744		76.18
	ATOM	795	N	ILE A		-9.534	42.797	47.322		42.69
	ATOM	796	CA	ILE A		-9.969	43.718	48.346		
60	ATOM	797	C	ILE A		-9.522				40.72
	ATOM	798	Ö	ILE A			45.167	48.099		46.21
	ATOM	799	СВ			-8.346 -0.570	45.478	47.866		42.68
				ILE A	104	-9.578	43.283	49.754		41.75
	ATOM	800		ILE A		-10.006	41.855	50.032		39.85
	MOTA	801	CGZ	ILE A	104	-10.225	44.222	50.768	1.00	41.53

	ATOM	802	CD1	ILE A 104	-8.839	40.995	50.485	1.00 34.17
	MOTA	803	N	SER A 105	-10.506	46.056	48.173	1.00 47.94
	ATOM	804	CA	SER A 105	-10.278	47.481	48.046	1.00 48.05
	ATOM	805	С	SER A 105	-10.184	47.977	49.482	1.00 42.39
5	ATOM	806	0	SER A 105	-11.134	47.879	50.263	1.00 39.69
	ATOM	807	CB	SER A 105	-11.399	48.180	47.290	1.00 53.77
	ATOM	808	OG	SER A 105	-11.399	47.789	45.930	1.00 60.69
	ATOM	809	N	PHE A 106	-9.020	48.445	49.857	1.00 35.07
10	ATOM	810	CA	PHE A 106	-8.844	48.890	51.223	1.00 34.98
10	MOTA	811	C	PHE A 106	-8.177	50.238	51.262	1.00 39.26
	ATOM	812	0	PHE A 106	-7.607	50.730	50.265	1.00 34.24
	ATOM	813	CB	PHE A 106	-8.015	47.864	52.060	1.00 36.05
	ATOM	814	CG	PHE A 106	-6.581	47.815	51.556	1.00 37.24
15	ATOM	815		PHE A 106	-6.251	47.073	50.422	1.00 39.71
15	ATOM	816		PHE A 106	-5.579	48.579	52.161	1.00 36.44
	ATOM	817 818		PHE A 106	-4.950	47.086	49.920	1.00 41.48
	MOTA MOTA	819	CZ	PHE A 106	-4.273	48.609	51.672	1.00 38.19
		820		PHE A 106	-3.961	47.856	50.540	1.00 37.91
20	ATOM ATOM	821	N CA	GLU A 107 GLU A 107	-8.284	50.794	52.453	1.00 40.64
40	ATOM	822	CA	GLU A 107 GLU A 107	-7.711	52.064	52.848	1.00 43.81
]= 4 0	ATOM	823	o		-7.206	51.869	54.284	1.00 43.82
i i i i i i i i i i i i i i i i i i i	ATOM	824	CB	GLU A 107	-7.933	51.303	55.121	1.00 38.38
\$20% (4.50)	ATOM	825	CG	GLU A 107 GLU A 107	-8.737	53.234	52.753	1.00 46.93
25	ATOM	826	CD	GLU A 107	-8.107	54.637	52.467	1.00 67.21
	ATOM	827		GLU A 107	-9.086	55.715	52.042	1.00100.00
ja £s	ATOM	828		GLU A 107	-10.208	55.504	51.599	1.00100.00
*	ATOM	829	N	THR A 108	-8.631 -5.963	56.938	52.221	1.00 93.72
-	ATOM	830	CA	THR A 108	-5.345	52.294	54.551	1.00 39.12
30	ATOM	831	C	THR A 108	-5.564	52.175 53.427	55.873	1.00 39.69
n.	ATOM	832	ŏ	THR A 108	-5.565		56.724	1.00 49.82
122	ATOM	833	СВ	THR A 108	-3.810	54.552 52.095	56.177 55.722	1.00 50.94
	ATOM	834	OG1	THR A 108	-3.360	53.226	54.981	1.00 40.40 1.00 32.22
	ATOM	835	CG2		-3.371	50.802	55.042	1.00 32.22
³⁵	ATOM	836	N	SER A 109	-5.698	53.217	58.065	1.00 40.43
	ATOM	837	CA	SER A 109	-5.848	54.294	59.038	1.00 42.02
	ATOM	838	С	SER A 109	-4.555	55.101	59.082	1.00 38.47
	ATOM	839	0	SER A 109	-3.460	54.583	58.921	1.00 33.60
	MOTA	840	CB	SER A 109	-6.166	53.759	60.437	1.00 41.44
40	ATOM	841	OG	SER A 109	-6.205	54.812	61.404	1.00 47.63
	ATOM	842	N	PRO A 110	-4.655	56.392	59.308	1.00 41.64
	ATOM	843	CA	PRO A 110	-3.419	57.116	59.393	1.00 40.75
	ATOM	844	С	PRO A 110	-2.803	56.749	60.725	1.00 41.47
4.5	ATOM	845	0	PRO A 110	-1.676	57.080	61.009	1.00 42.30
45	ATOM	846	CB	PRO A 110	-3.721	58.605	59.298	1.00 42.09
	ATOM	847	CG	PRO A 110	-5.224	58.719	59.132	1.00 48.77
	ATOM	848	CD	PRO A 110	-5.811	57.318	59.269	1.00 44.58
	ATOM	849	N	LYS A 111	-3.578	56.017	61.518	1.00 36.35
50	ATOM	850	CA	LYS A 111	-3.167	55.535	62.819	1.00 36.74
50	ATOM	851	C	LYS A 111	-2.669	54.083	62.720	1.00 40.19
	ATOM	852	0	LYS A 111	-2.733	53.319	63.678	1.00 40.53
	ATOM	853	CB	LYS A 111	-4.341	55.606	63.807	1.00 41.91
	ATOM	854	CG	LYS A 111	-4.362	56.838	64.708	1.00 71.21
55	ATOM	855	CD	LYS A 111	-5.421	57.854	64.309	1.00 97.95
23	ATOM	856	CE	LYS A 111	-6.839	57.394	64.611	1.00100.00
	ATOM	857	NZ	LYS A 111	-7.853	58.120	63.819	1.00100.00
	ATOM	858	N	SER A 112	-2.184	53.670	61.550	1.00 36.84
	ATOM	859	CA	SER A 112	-1.714	52.296	61.358	1.00 34.35
60	ATOM	860	C	SER A 112	-0.518	51.917	62.225	1.00 35.57
UU	ATOM	861	O	SER A 112	0.533	52.548	62.166	1.00 32.49
	ATOM	862	CB	SER A 112	-1.449	51.995	59.883	1.00 35.16
	ATOM	863	OG	SER A 112	-0.682	50.814	59.762	1.00 31.94
	ATOM	864 865	N	SER A 113	-0.666	50.872	63.033	1.00 31.84
	ATOM	865	CA	SER A 113	0.445	50.460	63.866	1.00 29.27

	MOTA	866	С	SER	Α	113	1.601	49.927	63.040	1 00	33.37
	MOTA	867	0	SER			2.715	49.792	63.497		32.95
	ATOM	868	CB	SER			0.052	49.498	64.945		29.45
	ATOM	869	OG	SER			0.032	48.169	64.462		34.27
5	ATOM	870	N	ALA			1.357	49.628			
	ATOM	871	CA	ALA			2.437	49.134	61.797		33.69
									60.981		34.05
	ATOM	872	С	ALA			3.239	50.287	60.388		37.83
	MOTA	873	0	ALA			4.411	50.149	60.033		37.72
10	MOTA	874	CB	ALA			1.845	48.292	59.852		34.51
10	ATOM	875	N	LEU			2.580	51.432	60.259	1.00	32.19
	ATOM	876	CA	LEU			3.201	52.595	59.662	1.00	30.48
	MOTA	877	С	LEU			3.509	53.745	60.565	1.00	35.32
	MOTA	878	0	LEU	Α	115	2.902	54.012	61.604		35.25
	ATOM	879	CB	LEU	Α	115	2.358	53.156	58.507		30.53
15	MOTA	880	CG	LEU	Α	115	1.787	52.064	57.602		35.51
	MOTA	881	CD1	LEU	A	115	0.812	52.710	56.637		35.12
	ATOM	882		LEU			2.903	51.387	56.821		33.88
de on	ATOM	883	N	GLN			4.490	54.457	60.096		34.00
	ATOM	884	CA	GLN			4.926	55.656	60.737		32.52
20	MOTA	885	C	GLN			5.066	56.689	59.645		
	ATOM	886	Ö	GLN			5.880	56.552-			31.34
h-A	ATOM	887	СВ	GLN			6.232				28.29
Ems.	ATOM	888	CG	GLN				55.540	61.496		32.66
क्ष्म् कर इस्	ATOM	889	CD	GLN			6.419	56.813	62.322		41.25
25							7.777	56.897	62.952		50.08
23	ATOM	890					8.515	55.905	63.017		55.36
1=40	ATOM	891		GLN			8.090	58.081	63.438		38.23
1	ATOM	892	N	TRP			4.210	57.680	59.748		26.66
5=£.	ATOM	893	CA	TRP			4.148	58.785	58.827		26.04
	ATOM	894	C	TRP			4.912	59.978	59.375		34.56
1,30	ATOM	895	0	TRP			4.467	60.589	60.364		36.83
T.	ATOM	896	CB	TRP			2.669	59.188	58.630		23.15
40 H	ATOM	897	CG	TRP			1.826	58.209	57.863		23.02
CD.	ATOM	898		TRP			1.052	57.224	58.397		26.39
35	ATOM	899		TRP			1.640	58.135	56.433		21.06
**** 33	ATOM	900		TRP			0.395	56.534	57.393	1.00	26.40
	ATOM	901		TRP			0.735	57.087	56.184		27.99
	ATOM	902		TRP			2.121	58.872	55.361	1.00	20.95
	MOTA	903		TRP			0.352	56.753	54.886		28.21
40	ATOM	904	CZ3				1.750	58.560	54.079	1.00	22.43
40	ATOM	905		TRP			0.872	57.512	53,847	1.00	24.28
	ATOM	906	N	LEU			6.043	60.340	58.756	1.00	31.44
	ATOM	907	CA	LEU			6.745	61.506	59.276	1.00	36.67
	ATOM	908	С	LEU			6.584	62.774	58.432		46.93
AE	ATOM	909	0	LEU			6.434	62.705	57.210	1.00	51.17
45	ATOM	910	CB	LEU			8.250	61.327	59.577	1.00	38.83
	ATOM	911	CG	LEU			8.881	59.939	59.398	1.00	44.33
	ATOM	912		LEU			10.392	60.065	59.569	1.00	42.12
	MOTA	913		LEU	А	118	8.351	58.950	60.426	1.00	49.99
- ^	ATOM	914	N	THR	Α	119	6.524	63.939	59.109		41.34
50	ATOM	915	CA	THR			6.449	65.260	58.468		38.89
	ATOM	916	С	THR	А	119	7.847	65.633	58.034		40.14
	ATOM	917	0	THR			8.841	65.165	58.605		44.03
	ATOM	918	CB	THR	Α	119	5.932	66.300	59.467		42.63
	ATOM	919	OG1	THR	Α	119	6.994	66.605	60.362		50.01
55	ATOM	920	CG2	THR	Α	119	4.769	65.668	60.224		36.78
	ATOM	921	N	PRO	Α	120	7.963	66.440	57.020		33.41
	MOTA	922	CA	PRO			9.275	66.781	56.517		33.18
	ATOM	923	С	PRO			10.260	67.209	57.599		38.27
	ATOM	924	0	PRO			11.433	66.829	57.566		34.42
60	ATOM	925	CB	PRO			9.068	67.840	55.416		33.54
	ATOM	926	CG	PRO			7.582	67.823	55.097		34.86
	ATOM	927	CD	PRO			6.891	67.180	56.300		30.86
	ATOM	928	N	GLU			9.751		58.563		38.03
	ATOM	929	CA	GLU			10.534	68.474	59.681		41.03
								-			

	ATOM	930	С	GLU A 121	11.2	12 67.361	60.411	1.00 50.88
	ATOM	931	0	GLU A 121	12.2	79 67.548	60.977	1.00 54.97
	ATOM	932	CB	GLU A 121	9.7		60.699	1.00 43.28
	ATOM	933	CG	GLU A 121	8.2			
5		934					60.702	1.00 64.72
,	ATOM		CD	GLU A 121	7.3		59.988	1.00 86.07
	ATOM	935	OE1		7.0	07 71.131	60.538	1.00100.00
	ATOM	936	OE2	GLU A 121	7.1	08 69.803	58.739	1.00 59.72
	ATOM	937	N	GLN A 122	10.5		60.394	1.00 44.09
	ATOM	938	CA	GLN A 122	11.0			
10	ATOM	939	C	GLN A 122			61.041	1.00 40.20
10					12.1		60.232	1.00 47.73
	ATOM	940	0	GLN A 122	12.7		60.643	1.00 53.29
	ATOM	941	СВ	GLN A 122	9.9	65 63.992	61.224	1.00 39.31
	ATOM	942	CG	GLN A 122	9.0	57 64.441	62.361	1.00 30.23
	MOTA	943	CD	GLN A 122	7.7		62.438	1.00 38.25
15	ATOM	944	OE1		6.8		61.548	
	ATOM	945	NE2					1.00 53.34
					7.5		63.521	1.00 18.98
	ATOM	946	N	THR A 123	12.4		59.074	1.00 38.99
	ATOM	947	CA	THR A 123	13.4	90 64.319	58.229	1.00 36.00
. 3%	ATOM	948	С	THR A 123	14.7	55 65.034	58.264	1.00 35.30
20	ATOM	949	0	THR A 123	14.8		58.875	1.00 34.95
43 20	ATOM	950	CB	THR A 123	13.0			
B=#A	ATOM	951	OG1				56.759	1.00 38.25
				THR A 123	13.1	-	56.046	1.00 43.75
ing the	ATOM	952	CG2		11.6	43 63.616	56.725	1.00 40.72
	ATOM	953	N	SER A 124	15.6	99 64.447	57.557	1.00 32.18
25	ATOM	954	CA	SER A 124	17.0	25 64.996	57.442	1.00 33.71
74 A R_H	ATOM	955	С	SER A 124	17.0		56.553	1.00 39.04
- #K	ATOM	956	0	SER A 124	17.5			
罪	ATOM	957	СВ	SER A 124			56.883	1.00 39.07
la fo					18.0		56.859	1.00 37.73
	ATOM	958	OG	SER A 124	18.3		57.796	1.00 36.28
30	ATOM	959	N	GLY A 125	16.3		55.414	1.00 38.59
T.	ATOM	960	CA	GLY A 125	16.2	80 67.034	54.396	1.00 39.90
	ATOM	961	С	GLY A 125	15.2		54.749	1.00 46.83
सेन कर्	ATOM	962	0	GLY A 125	15.3		54.172	
	ATOM	963	N	LYS A 126				1.00 49.78
35					14.3		55.678	1.00 41.09
33	ATOM	964	CA	LYS A 126	13.3		56.126	1.00 41.26
	ATOM	965	C	LYS A 126	12.4	98 69.307	55.020	1.00 47.42
	MOTA	966	0	LYS A 126	11.6	17 70.141	55.279	1.00 48.94
	ATOM	967	CB	LYS A 126	14.0	24 69.936	56.894	1.00 41.98
	ATOM	968	CG	LYS A 126	15.0		57.913	1.00 45.84
40	ATOM	969	CD	LYS A 126	14.5			
	ATOM	970	CE				59.135	1.00 58.74
				LYS A 126	15.6		60.151	1.00 72.12
	ATOM	971	NZ	LYS A 126	15.3		60.839	1.00 88.38
	MOTA	972	N	GLU A 127	12.7	22 68.858	53.792	1.00 41.82
	ATOM	973	CA	GLU A 127	11.9	21 69.344	52.708	1.00 41.98
45	ATOM	974	C	GLU A 127	10.8		52.239	1.00 45.14
	ATOM	975	0	GLU A 127	9.9		51.496	1.00 46.95
	ATOM	976	CB	GLU A 127	12.7		51.543	
	ATOM	977	CG	GLU A 127				1.00 44.39
	ATOM	978	CD		13.1		51.820	1.00 57.99
50				GLU A 127	12.3		51.301	1.00100.00
50	ATOM	979		GLU A 127	11.6		50.286	1.00100.00
	ATOM	980	OE2		12.3	87 73.758	52.054	1.00100.00
	ATOM	981	N	HIS A 128	11.0		52.653	1.00 39.18
	ATOM	982	CA	HIS A 128	10.0		52.210	1.00 39.43
	MOTA	983	С	HIS A 128	9.6			
55	ATOM	984					53.316	1.00 42.09
- 33			0	HIS A 128	10.3		54.281	1.00 45.34
	ATOM	985	СВ	HIS A 128	10.6		51.097	1.00 42.16
	MOTA	986	CG	HIS A 128	10.9	47 65.936	49.854	1.00 47.24
	ATOM	987	ND1	HIS A 128	9.9		49.029	1.00 49.12
	ATOM	988		HIS A 128	12.1		49.322	1.00 43.12
60	ATOM	989		HIS A 128	10.5			
	ATOM	990		HIS A 128			48.026	1.00 49.97
					11.8		48.166	1.00 50.87
	ATOM	991	N	PRO A 129	8.4		53.171	1.00 32.55
	ATOM	992	CA	PRO A 129	7.9		54.163	1.00 31.15
	ATOM	993	C	PRO A 129	8.6	36 62.328	53.900	1.00 34.90

	ATOM	994	0	PRO A 129	9.481	62.214	53.021	1.00 35.46
	MOTA	995	CB	PRO A 129	6.466	63.490	53.986	1.00 31.94
	ATOM	996	CG	PRO A 129	6.133	64.104	52.649	1.00 36.83
_	ATOM	997	CD	PRO A 129	7.384	64.850	52.185	1.00 32.71
5	ATOM	998	N	TYR A 130	8.248	61.342	54.659	1.00 29.47
	MOTA MOTA	999 1000	CA C	TYR A 130	8.826	60.025	54.548	1.00 29.35
	MOTA	1000	o	TYR A 130 TYR A 130	7.856 7.138	59.046	55.156	1.00 31.83
	ATOM	1001	СВ	TYR A 130	10.098	59.375 60.029	56.093 55.433	1.00 29.84
10	ATOM	1003	CG	TYR A 130	11.083	58.886	55.285	1.00 30.54 1.00 29.76
	ATOM	1004		TYR A 130	10.845	57.630	55.845	1.00 25.76
	ATOM	1005	CD2	TYR A 130	12.290	59.110	54.619	1.00 30.28
	ATOM	1006	CE1	TYR A 130	11.795	56.621	55.721	1.00 17.87
	MOTA	1007	CE2	TYR A 130	13.253	58.114	54.479	1.00 27.75
15	MOTA	1008	CZ	TYR A 130	12.983	56.866	55.031	1.00 25.76
	MOTA	1009	OH	TYR A 130	13.899	55.864	54.894	1.00 40.52
	ATOM	1010	N	LEU A 131	7.832	57.842	54.647	1.00 31.12
	ATOM	1011	CA	LEU A 131	6.994	56.868	55.303	1.00 30.43
	ATOM	1012	C	LEU A 131	7.691	55.568	55.289	1.00 33.91
20	ATOM ATOM	1013	0	LEU A 131	8.398	55.257	54.397	1.00 33.68
j	ATOM	1014 1015	CB CG	LEU A 131 LEU A 131	5.679	56.761	54.530	1.00 26.16
1=4	ATOM	1015		LEU A 131	5.065	55.367	54.600	1.00 21.68
अर्थे कर इस्स	ATOM	1017	CD2	LEU A 131	4.163	55.206	55.797	1.00 17.56
25	ATOM	1018	N	PHE A 132	7.533	55.008 54.828	53.380 56.348	1.00 13.86
	MOTA	1019	CA	PHE A 132	8.129	53.527	56.323	1.00 29.24 1.00 33.44
ļa£o,	ATOM	1020	C	PHE A 132	7.299	52.519	57.157	1.00 33.44
*	ATOM	1021	Ō	PHE A 132	6.344	52.889	57.837	1.00 41.08
	ATOM	1022	CB	PHE A 132	9.621	53.670	56.791	1.00 36.40
30	ATOM	1023	CG	PHE A 132	9.763	53.895	58.256	1.00 38.11
nj	MOTA	1024	CD1	PHE A 132	9.601	52.821	59.053	1.00 37.18
	ATOM	1025	CD2		10.123	55.158	58.803	1.00 43.89
25	ATOM	1026		PHE A 132	9.771	52.936	60.422	1.00 41.04
25	ATOM	1027	CE2	PHE A 132	10.289	55.258	60.174	1.00 47.72
_⊫ "35	ATOM	1028	CZ	PHE A 132	10.131	54.143	60.986	1.00 44.34
	ATOM ATOM	1029 1030	N CA	SER A 133 SER A 133	7.612	51.221	57.002	1.00 33.47
	ATOM	1030	CA	SER A 133	6.744	50.228	57.629	1.00 29.86
	ATOM	1031	Ö	SER A 133	7.499 8.724	49.221 49.146	58.504 58.531	1.00 31.53
40	ATOM	1033	СВ	SER A 133	5.942	49.481	56.535	1.00 33.16 1.00 33.19
	ATOM	1034	OG	SER A 133	6.757	48.480	55.926	1.00 50.66
	ATOM	1035	N	GLN A 134	6.703	48.466	59.294	1.00 30.00
	ATOM	1036	CA	GLN A 134	7.283	47.422	60.134	1.00 22.55
	ATOM	1037	С	GLN A 134	6.268	46.321	60.398	1.00 27.28
45	ATOM	1038	0	GLN A 134	5.161	46.566	60.809	1.00 25.09
	ATOM	1039	СВ	GLN A 134	7.711	48.041	61.464	1.00 23.29
	ATOM	1040	CG	GLN A 134	8.218	46.987	62.454	1.00 25.96
	ATOM	1041	CD	GLN A 134	9.423	46.290	61.872	1.00 25.65
50	ATOM ATOM	1042 1043	OE1 NE2	GLN A 134	10.296	46.876	61.263	1.00 26.36
.50	ATOM	1043	N	GLN A 134 CYS A 135	9.445	44.965	62.095	1.00 21.75
	ATOM	1045	CA	CYS A 135	6.435 5.291	45.124 44.220	59.820	1.00 29.60
	ATOM	1046	C	CYS A 135	5.442	43.006	59.755 60.662	1.00 32.30 1.00 39.58
	ATOM	1047	o	CYS A 135	4.597	42.144	60.739	1.00 39.38
55	ATOM	1048	CB	CYS A 135	5.098	43.794	58.320	1.00 40.94
	ATOM	1049	SG	CYS A 135	3.976	44.922	57.445	1.00 33.40
	MOTA	1050	N	GLN A 136	6.582	42.949	61.345	1.00 37.37
	ATOM	1051	CA	GLN A 136	6.715	41.982	62.417	1.00 35.71
-	ATOM	1052	С	GLN A 136	6.589	42.645	63.797	1.00 31.90
60	ATOM	1053	0	GLN A 136	6.878	43.803	63.981	1.00 30.54
	ATOM	1054	CB	GLN A 136	8.077	41.311	62.295	1.00 37.24
	ATOM	1055	CG	GLN A 136	8.076	39.878	62.847	1.00 29.70
	ATOM	1056	CD	GLN A 136	9.483	39.511	63.235	1.00 36.48
	MOTA	1057	OFI	GLN A 136	10.366	40.328	63.356	1.00 24.49

	ATOM	1058	NE2	GLN A	136	9.665	38.201	63.443	1.00	22.19
	ATOM	1059	N	ALA A		5.850	41.899	64.648		28.56
	MOTA	1060	CA	ALA A	137	5.235	40.581	64.351		28.89
	MOTA	1061	С	ALA A	137	3.860	40.503	63.630		31.83
5	MOTA	1062	0	ALA A	137	3.679	39.688	62.738		29.67
	ATOM	1063	CB	ALA A	137	5.091	39.742	65.625		28.91
	ATOM	1064	N	ILE A		2.863	41.285	64.070		27.07
	ATOM	1065	CA	ILE A		1.553	41.176	63.445		23.90
. 10	ATOM	1066	С	ILE A		0.960	42.492	63.053		28.69
10	ATOM	1067	0	ILE A		-0.144	42.822	63.426	1.00	31.92
	MOTA	1068	CB	ILE A		0.641	40.357	64.339	1.00	25.41
	ATOM	1069		ILE A		0.871	40.811	65.801	1.00	27.32
	MOTA	1070	CG2			1.162	38.938	64.191	1.00	16.34
15	ATOM	1071		ILE A		-0.275	40.615	66.826		20.22
13	MOTA	1072 1073	n Ca	HIS A		1.718	43.223	62.265		24.05
	ATOM ATOM	1073	CA	HIS A		1.322	44.511	61.824		24.05
	ATOM	1074	0	HIS A		0.982	44.579	60.351		34.40
	ATOM	1076	СВ	HIS A		0.539	45.625	59.888		35.89
20	ATOM	1077	CG	HIS A		2.439 2.689	45.519	62.173		24.63
	ATOM	1078		HIS A		1.679	45.619	63.657		27.97
ja.	ATOM	1079		HIS A		3.835	45.970 45.437	64.571		27.75
अर्च सार्थ इंड्स	ATOM	1080		HIS A		2.222	45.983	64.356 65.770		28.42
17 19 19 19 19 19 19 19 19 19 19 19 19 19	ATOM	1081		HIS A		3.517	45.668	65.671		26.19
25	ATOM	1082	N	CYS A		1.181	43.490	59.598		27.42 30.28
23	ATOM	1083	CA	CYS A		0.832	43.517	58.181		28.08
ļ.	ATOM	1084	С	CYS A		-0.671	43.765	58.011		28.98
琊	MOTA	1085	0	CYS A		-1.111	44.449	57.066		30.00
j=#.	ATOM	1086	CB	CYS A		1.181	42.213	57.447		28.82
1. 30	MOTA	1087	SG	CYS A	140	1.330	42.483	55.661		34.37
n.	MOTA	1088	N	ARG A	141	-1.440	43.168	58.949		20.78
14 H	MOTA	1089	CA	ARG A		-2.884	43.252	58.996		20.33
12 m	MOTA	1090	С	ARG A		-3.286	44.684	59.003		32.37
35	ATOM	1091	0	ARG A		-4.355	45.032	58.510		35.81
F 33	ATOM	1092	СВ	ARG A		-3.557	42.498	60.156	1.00	14.60
	ATOM	1093	CG	ARG A		-3.081	42.891	61.568	1.00	20.94
	ATOM	1094	CD	ARG A		-3.576	41.978	62.715	1.00	19.99
	ATOM	1095	NE	ARG A		-2.911	40.690	62.786		18.24
40	ATOM ATOM	1096 1097	CZ	ARG A		-3.140	39.707	63.648		18.77
70	ATOM	1097		ARG A		-4.029	39.739	64.634		20.76
	ATOM	1090	NH2	ALA A		-2.415 -2.408	38.640	63.508		24.20
	ATOM	1100	CA	ALA A		-2.668	45.511 46.940	59.580		28.35
	ATOM	1101	C	ALA A		-2.369	47.652	59.657 58.345		27.60
45	ATOM	1102	O	ALA A		-2.620	48.835	58.203		34.33
	ATOM	1103	СВ	ALA A		-1.994	47.616	60.843		27.67
	ATOM	1104	N	ILE A		-1.824	46.922	57.382		32.39
	MOTA	1105	CA	ILE A	143	-1.537	47.499	56.099		30.38
50	ATOM	1106	С	ILE A		-2.520	46.994	55.067		37.79
50	ATOM	1107	0	ILE A		-2.885	47.709	54.152		42.65
	ATOM	1108	CB	ILE A		-0.142	47.228	55.613		32.06
	ATOM	1109		ILE A		0.827	48.062	56.414		31.71
	ATOM	1110		ILE A		-0.074	47.654	54.143	1.00	34.02
55	ATOM	1111		ILE A		2.258	47.774	55.988		42.10
در	ATOM	1112	N	LEU A		-2.939	45.749	55.218		32.50
	ATOM	1113		LEU A		-3.873	45.142	54.291		32.36
	ATOM ATOM	1114		LEU A		-4.435	43.838	54.849		40.36
	ATOM	1115 1116		LEU A		-3.959	43.278	55.852		33.27
60	ATOM	1117		LEU A		-3.250	44.936	52.894		31.58
	ATOM	1117	CD1	LEU A	144	-1.923	44.170	52.917		33.31
	ATOM	1119		LEU A		-2.147 -0.836	42.770	52.352		32.07
	ATOM	1120		PRO A		-5.490	44.897	52.110		28.67
	ATOM	1121		PRO A		-6.080	43.347 42.129	54.213 54.715		40.02
		-					32.127	34.113	T.00	37.86

	ATOM	1122	С	PRO A 145		-5.264	40.941	54.286	1.00 37.87
	ATOM	1123	0	PRO A 145		-4.819	40.831	53.144	
	ATOM	1124	СВ	PRO A 145		-7.530	42.080	54.220	1.00 35.27
	ATOM	1125	CG	PRO A 145		-7.778			1.00 38.81
5	ATOM	1126	CD	PRO A 145			43.393	53.492	1.00 41.34
		1127				-6.432	44.093	53.341	1.00 36.69
	ATOM		N	CYS A 146		-5.041	40.056	55.233	1.00 36.18
	ATOM	1128	CA	CYS A 146	•	-4.250	38.882	54.958	1.00 35.60
	MOTA	1129	С	CYS A 146		-4.358	37.859	56.069	1.00 33.04
10	ATOM	1130	0	CYS A 146		-5.067	38.062	57.050	1.00 30.78
10	ATOM	1131	CB	CYS A 146		-2.761	39.287	54.813	1.00 36.08
	ATOM	1132	SG	CYS A 146		-2.087	40.108	56.302	1.00 39.43
	ATOM	1133	N	GLN A 147		-3.637	36.755	55.883	1.00 29.33
	ATOM	1134	CA	GLN A 147		-3.517	35.703	56.875	1.00 29.71
	MOTA	1135	С	GLN A 147		-2.254	36.131	57.628	1.00 29.71
15	MOTA	1136	Ō	GLN A 147		-1.141	35.926	57.135	
	ATOM	1137	СВ	GLN A 147		-3.322			1.00 40.79
	ATOM	1138	CG			-	34.352	56.206	1.00 28.99
and the control of th	ATOM	1139	CD	GLN A 147		-4.672	33.707	55.894	1.00 25.73
C)				GLN A 147		-4.562	32.532	54.960	1.00 39.92
20	ATOM	1140	OE1			-4.217	32.668	53.775	1.00 43.89
41 20 T	ATOM	1141	NE2			-4.828	31.368	55.499	1.00 26.36
Jak.	ATOM	1142	N	ASP A 148		-2.425	36.834	58.765	1.00 32.68
	MOTA	1143	CA	ASP A 148		-1.287	37.362	59.474	1.00 33.50
	ATOM	1144	С	ASP A 148		-0.629	36.377	60.371	1.00 33.13
HERE	ATOM	1145	0	ASP A 148		-0.622	36.563	61.584	1.00 33.13
25	ATOM	1146	СВ	ASP A 148		-1.633	38.642	60.253	
J.A.	ATOM	1147	CG	ASP A 148		-0.535	39.666		1.00 37.78
	ATOM	1148		ASP A 148		0.564		60.332	1.00 45.10
2	ATOM	1149	003	ASP A 148			39.540	59.836	1.00 47.89
]=#.	ATOM	1150	N			-0.913	40.737	60.952	1.00 48.63
30	ATOM			THR A 149		-0.080	35.345	59.742	1.00 29.15
n s		1151	CA	THR A 149		0.584	34.251	60.422	1.00 28.25
11 '41'- 12 '41'-	ATOM	1152	C	THR A 149		1.805	33.831	59.625	1.00 34.92
	ATOM	1153	0	THR A 149		1.757	33.764	58.410	1.00 34.47
121	ATOM	1154	CB	THR A 149		-0.403	33.087	60.674	1.00 24.79
¹⁼¹ 35	ATOM	1155	OG1			0.241	32.059	61.352	1.00 37.15
35	ATOM	1156	CG2	THR A 149		-0.905	32.527	59.345	1.00 26.56
	ATOM	1157	N	PRO A 150		2.910	33.575	60.323	1.00 34.69
	ATOM	1158	CA ·	PRO A 150		4.142	33.217	59.659	1.00 31.06
	ATOM	1159	С	PRO A 150		4.087	31.813	59.131	1.00 36.66
	ATOM	1160	0	PRO A 150		4.995	31.356	58.450	1.00 36.37
40	ATOM	1161	CB	PRO A 150		5.245	33.327	60.712	1.00 30.37
	ATOM	1162	CG	PRO A 150		4.570	33.471	62.077	1.00 36.95
	ATOM	1163	CD	PRO A 150		3.078	33.589	61.823	
	ATOM	1164	N	SER A 151		2.992	31.150	59.452	1.00 34.62
	ATOM	1165	CA	SER A 151		2.778			1.00 31.62
45	MOTA	1166	C	SER A 151			29.791	59.029	1.00 27.35
	ATOM	1167	Ö	SER A 151		2.357	29.738	57.564	1.00 32.97
	ATOM	1168	СВ			2.344	28.703	56.928	1.00 34.25
	ATOM			SER A 151		1.714	29.203	59.905	1.00 25.95
		1169	OG	SER A 151		0.483	29.685	59.439	1.00 49.35
50	ATOM	1170	N	VAL A 152		1.997	30.887	57.024	1.00 34.36
50	ATOM	1171	CA	VAL A 152		1.595	31.015	55.623	1.00 33.74
	ATOM	1172	С	VAL A 152		2.705	31.764	54.847	1.00 37.45
	ATOM	1173	0	VAL A 152		3.295	32.761	55.313	1.00 37.63
	ATOM	1174	CB	VAL A 152		0.203	31.697	55.427	1.00 32.61
	MOTA	1175	CG1	VAL A 152		-0.184	31.767	53.963	1.00 31.50
55	ATOM	1176	CG2	VAL A 152		-0.915	30.975	56.149	1.00 31.29
	ATOM	1177	N	LYS A 153		2.999	31.289	53.654	1.00 26.98
	ATOM	1178	CA	LYS A 153		4.002	31.927	52.866	
	ATOM	1179	c c	LYS A 153		3.469			1.00 25.81
	ATOM	1180	Ö	LYS A 153			32.141	51.473	1.00 33.94
60	ATOM	1181	СВ	LYS A 153		2.826	31.251	50.936	1.00 32.91
	ATOM					5.252	31.091	52.841	1.00 24.70
		1182	CG	LYS A 153		6.383	31.760	53.583	1.00 34.68
	ATOM	1183	CD	LYS A 153		7.641	30.893	53.616	1.00 39.37
	ATOM	1184	CE	LYS A 153		8.121	30.506	55.015	1.00 29.09
	ATOM	1185	NZ	LYS A 153		9.556	30.152	55.112	1.00 26.03

	ATOM	1186	N	LEU A	154	3.732	33.321	50.896	1.00 32.13
	ATOM	1187	CA	LEU A		3,285	33.639		
								49.544	1.00 30.67
	ATOM	1188	С	LEU A	154	4.279	34.475	48.789	1.00 40.67
	ATOM	1189	0	LEU A	154	5.264	35.000	49.344	1.00 42.56
5	ATOM	1190	СВ	LEU A					
,						1.966	34.432	49.515	1.00 30.10
	MOTA	1191	CG	LEU A	154	2.084	35.793	50.207	1.00 35.20
	MOTA	1192	CD1	LEU A	154	0.989	36.716		
								49.690	1.00 37.21
	ATOM	1193	CD2	LEU A	154	1.934	35.608	51.715	1.00 33.07
	ATOM	1194	N	THR A	155	3.963	34.610	47.499	1.00 37.82
10	ATOM	1195	CA	THR A					
10						4.728	35.449	46.596	1.00 38.44
	ATOM	1196	С	THR A	155	3.934	36.730	46.389	1.00 41.52
	ATOM	1197	0	THR A		2.738	36.775	46.674	
									1.00 43.95
	MOTA	1198	CB	THR A		5.041	34.814	45.230	1.00 36.99
	ATOM	1199	OG1	THR A	155	3.886	34.281	44.584	1.00 32.59
15	ATOM	1200	CG2						
13						6.133	33.790	45.404	1.00 18.24
	ATOM	1201	N	TYR A	156	4.563	37.768	45.892	1.00 33.87
	ATOM	1202	CA	TYR A	156	3.835	39.003		
								45.683	1.00 32.49
	ATOM	1203	С	TYR A		4.509	39.922	44.717	1.00 37.91
	ATOM	1204	0	TYR A	156	5.725	39.940	44.562	1.00 39.04
20	ATOM	1205	CB	TYR A					
20						3.534	39.795	46.983	1.00 31.16
	ATOM	1206	CG	TYR A	156	4.642	40.731	47.471	1.00 28.94
	ATOM	1207	CD1	TYR A	156	4.817	42.021	46.969	
-									1.00 30.33
	MOTA	1208	CD2		156	5.525	40.303	48.465	1.00 30.43
	ATOM	1209	CE1	TYR A	156	5.829	42.853	47.459	1.00 36.89
25	ATOM	1210	CE2						
						6.553	41.104	48.960	1.00 31.47
	ATOM	1211	cz	TYR A	156	6 .6 90	42.396	48.462	1.00 43.34
	ATOM	1212	OH	TYR A	156	7.701	43.180	48.956	1.00 36.86
	ATOM								
		1213	N	THR A		3.657	40.689	44.101	1.00 36.75
	ATOM	1214	CA	THR A	157	4.036	41.691	43.171	1.00 38.49
30	ATOM	1215	С	THR A	157	3.346	42.942	43.611	
									1.00 42.61
	ATOM	1216	0	THR A		2.228	42.913	44.143	1.00 38.45
	ATOM	1217	CB	THR A	157	3.631	41.316	41.751	1.00 39.73
	ATOM	1218	OG1	THR A		2.380			
							40.655	41.803	1.00 55.71
~-	ATOM	1219	CG2			4.680	40.370	41.212	1.00 26.71
35	ATOM	1220	N	ALA A	158	4.037	44.025	43.404	1.00 41.36
	ATOM	1221	CA	ALA A					
						3.488	45.273	43.789	1.00 41.08
*	ATOM	1222	С	ALA Ą	158	3.869	46.401	42.839	1.00 50.77
	ATOM	1223	0	ALA A	158	4.919	46.390	42.179	1.00 53.47
	ATOM	1224	СВ	ALA A					
40						3.910	45.570	45.212	1.00 39.87
40	MOTA	1225	N	GLU A	159	2.974	47.376	42.788	1.00 43.90
	ATOM	1226	CA	GLU A	159	3.107	48.604	42.023	1.00 42.27
	ATOM	1227	С	GLU A					
						2.451	49.705	42.843	1.00 42.17
	ATOM	1228	0	GLU A	159	1.257	49.630	43.227	1.00 41.00
	ATOM	1229	CB	GLU A	159	2.641	48.521	40.571	1.00 43.72
45									
30	ATOM	1230	CG	GLU A			47.197	40.255	1.00 62.90
	ATOM	1231	CD	GLU A	159	1.502	47.156	38.835	1.00 91.28
	ATOM	1232	OF.1	GLU A		2.202	46.696	37.955	
									1.00 77.84
	MOTA	1233		GLU A		0.322	47.707	38.644	1.00100.00
	ATOM	1234	N	VAL A	160	3.263	50.686	43.197	1.00 34.67
50	ATOM	1235	CA	VAL A					
-						2.738	51.717	44.044	1.00 36.57
	ATOM	1236	С	VAL A	160	3.024	53.091	43.533	1.00 43.02
	ATOM	1237	0	VAL A	160	4.121	53.380	43.050	1.00 42.71
	ATOM	1238	CB						
				VAL A		3.180	51.530	45.500	1.00 40.73
	MOTA	1239		VAL A		3.988	50.239	45.644	1.00 38.56
55	MOTA	1240		VAL A		4.006	52.728	45.963	
									1.00 40.46
	ATOM	1241	N	SER A		2.002	53.922	43.653	1.00 41.79
	MOTA	1242	CA	SER A	161	2.076	55.292	43.185	1.00 42.07
	ATOM	1243	С	SER A					
						2.532	56.204	44.270	1.00 44.28
60	ATOM	1244	0	SER A	101	2.047	56.121	45.403	1.00 43.60
60	ATOM	1245	CB	SER A	161	0.751	55.801	42.635	1.00 43.32
	ATOM	1246	OG	SER A		0.971			
							56.850	41.726	1.00 49.40
	MOTA	1247	N.	VAL A		3.447	57.080	43.896	1.00 36.49
	ATOM	1248	CA	VAL A	162	3.979	58.019	44.838	1.00 34.99
	ATOM	1249	С	VAL A	T 07	4.273	59.319	44.148	1.00 42.57

	ATOM	1250	0	VAL	Α	162	4.470	59.354	42.932	1.00 44.41
	ATOM	1251	CB	VAL			5.300	57.498	45.402	1.00 35.97
	ATOM	1252	CG1	VAL			5.084	56.219	46.188	1.00 36.12
_	MOTA	1253	CG2	VAL	Α	162	6.222	57.194	44.239	1.00 35.42
5	MOTA	1254	N	PRO	Α	163	4.332	60.377	44.942	1.00 32.95
	ATOM	1255	CA	PRO			4.664	61.662	44.400	1.00 31.07
	ATOM	1256	С	PRO			5.966	61.496	43.652	1.00 39.67
	MOTA	1257	0	PRO .			6.919	60.892	44.142	1.00 42.78
10	MOTA	1258	CB	PRO			4.780	62.562	45.618	1.00 31.62
10	ATOM	1259	CG	PRO			3.946	61.893	46.714	1.00 33.93
	MOTA	1260	CD	PRC			3.652	60.480	46.259	1.00 28.53
	MOTA	1261	N	LYS			5.962	61.978	42.436	1.00 38.52
	ATOM	1262	CA	LYS			7.086	61.860	41.539	1.00 39.97
15	ATOM	1263	C	LYS .			8.451	62.222	42.088	1.00 42.75
15	ATOM	1264	0	LYS .			9.453	61.708	41.593	1.00 44.47
	ATOM	1265	CB	LYS .			6.828	62.479	40.177	1.00 44.67
	ATOM	1266	CG	LYS .			6.004	63.758	40.257	1.00 78.05
	ATOM	1267	CD	LYS .			6.651	64.918	39.497	1.00100.00
20	ATOM	1268	CE	LYS .			6.016	66.289	39.772	1.00100.00
15.0	ATOM	1269	NZ	LYS .			6.679	67.075	40.835	1.00100.00
j.k	ATOM	1270	N	GLU .			8.519	63.097	43.082	1.00 37.25
# 12 PR/ 12 PR/	ATOM ATOM	1271	CA	GLU .			9.814	63.489	43.665	1.00 39.56
9 9Rk.	ATOM	1272 1273	C	GLU .			10.333	62.462	44.677	1.00 46.39
25	ATOM	1273	O CB	GLU .			11.531	62.318	44.927	1.00 48.93
	ATOM	1275	CG	GLU .			9.797	64.902	44.297	1.00 42.10
ja 44	ATOM	1276	CD	GLU .			8.602	65.156	45.257	1.00 58.16
B	ATOM	1277	OE1				7.214	64.970	44.664	1.00 88.01
B=#(ATOM	1278	OE2				6.994 6.266	64.757	43.475	1.00 79.46
1.30	ATOM	1279	N	LEU .			9.398	65.050	45.575	1.00 70.27
	ATOM	1280	CA	LEU			9.696	61.733 60.733	45.265	1.00 40.39
E-10	ATOM	1281	C	LEU			9.934	59.377	46.254 45.640	1.00 36.56
्रद्र म _{्रि}	ATOM	1282	0	LEU			9.366	59.080	44.581	1.00 47.57 1.00 52.86
##\ ##	ATOM	1283	CB	LEU			8.525	60.630	47.250	1.00 32.86
35	ATOM	1284	CG	LEU .			8.315	61.912	48.057	1.00 31.92
	MOTA	1285	CD1	LEU	A	166	7.363	61.590	49.189	1.00 25.96
	ATOM	1286		LEU I			9.635	62.467	48.622	1.00 23.78
	ATOM	1287	N	VAL :	Α	167	10.769	58.564	46.328	1.00 34.75
	ATOM	1288	CA	VAL I	A	167	11.077	57.218	45.908	1.00 30.00
40	MOTA	1289	С	VAL 3	A	167	10.332	56.229	46.771	1.00 38.80
	MOTA	1290	0	VAL I			9.902	56.532	47.879	1.00 40.91
	ATOM	1291	CB	VAL J			12.549	56.860	46.048	1.00 31.28
	ATOM	1292	CG1				12.854	55.542	45.329	1.00 28.20
AE	ATOM	1293		VAL 1			13.456	57.964	45.565	1.00 31.06
45	ATOM	1294	N	ALA I			10.217	55.019	46.257	1.00 36.46
	ATOM	1295	CA	ALA I			9.584	53.935	46.979	1.00 35.14
	ATOM	1296	C	ALA I			10.418	52.662	46.836	1.00 43.27
	ATOM	1297	O	ALA I			10.889	52.343	45.733	1.00 44.74
50	ATOM ATOM	1298 1299	CB	ALA A			8.149	53.700	46.550	1.00 34.20
50	ATOM	1300	N CA	LEU I			10.603	51.960	47.975	1.00 35.27
	ATOM	1300	CA	LEU A			11.323	50.696	48.069	1.00 29.39
	ATOM	1302	0	LEU A			10.491	49.635	48.797	1.00 33.87
	ATOM	1303	СВ	LEU I			9.604	49.918	49.613	1.00 31.21
55	ATOM	1304	CG	LEU I			12.721 13.593	50.835	48.656	1.00 28.62
	ATOM	1305		LEU A			14.953	51.810	47.891	1.00 35.90
	ATOM	1306		LEU A			13.765	51.819	48.558	1.00 39.38
	ATOM	1307	N	MET A			10.758	51.394 48.381	46.432 48.479	1.00 37.35
	ATOM	1308	CA	MET A			10.738	47.291		1.00 34.23
60	ATOM	1309	C	MET A			10.874	46.083	49.069 49.287	1.00 31.07
	ATOM	1310	ō	MET 7			11.995	45.973	48.775	1.00 34.13 1.00 35.20
	ATOM	1311	CB	MET 7			8.842	46.882	48.154	1.00 35.20
	ATOM	1312	CG	MET A			7.751	47.934	48.116	1.00 31.95
	ATOM	1313	SD	MET A			6.105	47.253	47.815	1.00 34.54

	ATOM	1314	CE	MET A	170	5.820	46.349	49.363	1.00 32.25
	ATOM	1315	N	SER A	171	10.332	45.165	50.057	1.00 28.20
	ATOM	1316	CA	SER A		11.064	43.953	50.297	1.00 28.47
	ATOM	1317	C	SER A		10.929	43.054	49.049	1.00 32.01
5	ATOM	1318	0	SER A		10.396	41.958	49.089	1.00 30.93
	ATOM	1319	CB	SER A	171	10.662	43.265	51.606	1.00 30.93
	ATOM	1320	OG	SER A	171	9.297	42.920	51.581	1.00 32.90
	ATOM	1321	N	ALA A	172	11.401	43.543	47.912	1.00 28.84
	ATOM	1322	CA	ALA A		11.286	42.773		
10								46.691	1.00 29.48
10	MOTA	1323	С	ALA A		12.241	43.258	45.644	1.00 37.63
	MOTA	1324	0	ALA A		13.060	44.147	45.881	1.00 35.07
	ATOM	1325	CB	ALA A	172	9.884	42.969	46.120	1.00 29.48
	ATOM	1326	N	ILE A	173	12.104	42.686	44.452	1.00 39.49
	ATOM	1327	CA	ILE A		12.966	43.120	43.382	1.00 38.64
15	ATOM	1328	c.	ILE A					
13						12.418	44.343	42.648	1.00 44.83
	MOTA	1329	0	ILE A		11.269	44.394	42.193	1.00 40.97
· · · · · · · · · · · · · · · · · · ·	ATOM	1330	CB	ILE A		13.549	42.027	42.479	1.00 38.79
	ATOM	1331	CG1	ILE A	173	14.258	40.970	43.302	1.00 37.40
u D	ATOM	1332	CG2	ILE A	173	14.606	42.621	41.570	1.00 38.88
20	MOTA	1333		ILE A		15.770	41.069	43.193	1.00 25.93
## ~ 0		1334	N						
]= 4 5,	ATOM			ARG A		13.286	45.345	42.584	1.00 43.21
340	ATOM	1335	CA	ARG A		12.997	46.567	41.917	1.00 42.34
· 明春秋/ 明春秋/	ATOM	1336	С	ARG A		12.630	46.173	40.516	1.00 47.54
· · · · · · · · · · · · · · · · · · ·	ATOM	1337	0	ARG A	174	13.478	45.667	39.770	1.00 42.08
25	ATOM	1338	CB	ARG A	174	14.254	47.422	41.937	1.00 42.47
j= # ₀	ATOM	1339	CG	ARG A		14.231	48.450	43.075	1.00 53.40
*	MOTA	1340	CD	ARG A	-				
100						15.617	48.917	43.515	1.00 33.80
 - 4 .	MOTA	1341	NE	ARG A		16.036	50.083	42.756	1.00 53.32
30	MOTA	1342	CZ	ARG A		17.221	50.208	42.181	1.00 97.11
30	ATOM	1343	NH1	ARG A	174	18.132	49.243	42.266	1.00100.00
	MOTA	1344	NH2	ARG A	174	17.503	51.321	41.489	1.00100.00
(**) (**)	ATOM	1345	N	ASP A		11.356	46.356	40.195	1.00 51.12
		1346		ASP A					
	ATOM		CA			10.858	45.981	38.882	1.00 53.89
	ATOM	1347	С	ASP A		10.778	47.128	37.885	1.00 58.32
35	MOTA	1348	0	ASP A		10.455	46.901	36.727	1.00 56.00
	ATOM	1349	CB	ASP A	175	9.533	45.186	38.948	1.00 57.16
	ATOM	1350	CG	ASP A	175	9.196	44.446	37.675	1.00 81.25
	ATOM	1351	OD1	ASP A		10.034	44.118	36.851	1.00 83.53
	ATOM	1352		ASP A		7.910	44.176		
40								37.558	1.00 92.45
40	ATOM	1353	N	GLY A		11.062	48.356	38.331	1.00 58.24
	ATOM	1354	CA	GLY A		11.021	49.498	37.438	1.00 57.71
	ATOM	1355	С	GLY A	176	9.969	50.546	37.773	1.00 58.98
	MOTA	1356	0	GLY A	176	9.090	50.371	38.620	1.00 52.04
	ATOM	1357	N	GLU A	177	10.110	51.649	37.050	1.00 63.72
45	ATOM	1358	CA	GLU A		9.267	52.812	37.172	1.00 67.79
	ATOM	1359	С	GLU A		8.874			
	ATOM	1360	Õ	GLU A			53.388	35.817	1.00 86.22
						9.614	53.364	34.830	1.00 91.14
	ATOM	1361	CB	GLU A		9.986	53.902	38.006	1.00 68.25
~ ^	MOTA	1362	CG	GLU A		11.432	54.145	37.519	1.00 71.58
50	ATOM	1363	CD	GLU A	177	12.183	55.088	38.404	1.00 85.08
	MOTA	1364	OE1	GLU A	177	13.045	54.733	39.198	1.00100.00
	ATOM	1365		GLU A		11.765	56.316	38.264	
	ATOM	1366	N	THR A					1.00 56.71
						7.671	53.924	35.835	1.00 84.76
	ATOM	1367	CA	THR A	`	6.684	54.686	35.042	1.00 84.81
55	ATOM	1368	С	THR A		6.024	55.810	35.855	1.00 90.37
	ATOM	1369	0	THR A	178	5.664	55.655	36.996	1.00 91.10
	ATOM	1370	СВ	THR A		5.618	53.713	34.561	1.00 89.82
	ATOM	1371		THR A		5.283	52.830	35.636	
									1.00 80.25
60	ATOM	1372		THR A		6.161	52.898	33.396	1.00 93.46
60	MOTA	1373	N	PRO A		5.921	56.984	35.217	1.00 87.05
	ATOM	1374	CA	PRO A		5.365	58.187	35.845	1.00 86.61
	ATOM	1375	С	PRO A	179	3.857	58.419	35.531	1.00 89.04
	MOTA	1376	0	PRO A		3.444	59.516	35.140	1.00 91.15
	MOTA	1377	CB	PRO A		6.176	59.345	35.301	1.00 88.63
							22.23		

	MOTA	1378	CG	PRO A	179	6.657	58.947	33.895	1.00 92.62
	ATOM	1379	CD	PRO A		6.426	57.345	33.902	1.00 87.63
	MOTA	1380	N	ASP A		3.020	57.347	35.694	1.00 82.31
	ATOM	1381	CA	ASP A		1.616	57.568	35.310	1.00 81.19
5	ATOM	1382	С	ASP A		0.629	56.743	36.166	1.00 90.72
	ATOM	1383	0	ASP A		0.533	55.519	36.072	1.00 91.13
	MOTA	1384	CB	ASP A		1.458	57.196	33.827	1.00 82.12
	ATOM	1385	CG	ASP A		0.087	57.651	33.327	1.00 95.94
10	ATOM	1386		ASP A		-0.155	58.858	33.337	1.00100.00
10	ATOM	1387		ASP A		-0.714	56.801	32.946	1.00 94.36
	ATOM	1388 1389	N CA	PRO A		-0.060	57.456	37.086	1.00 92.45
	MOTA MOTA	1390	C	PRO A		-1.212 -2.519	56.934 57.566	37.795 37.284	1.00 92.02
	ATOM	1391	0	PRO A		-2.605	58.114	36.192	1.00100.00
15	ATOM	1392	СВ	PRO A		-1.014	57.340	39.210	1.00 92.48
13	ATOM	1393	CG	PRO A		-0.362	58.734	39.152	1.00 92.48
	ATOM	1394	CD	PRO A		0.268	58.736	37.663	1.00 94.17
-17 to).	ATOM	1395	N	GLU A		-3.567	57.456	38.141	1.00100.00
	ATOM	1396	CA	GLU A		-4.822	58.161	37.876	1.00 98.21
20	MOTA	1397	С	GLU A		-5.359	58.856	39.154	1.00100.00
	ATOM	1398	0	GLU A	182	-6.404	59.497	39.167	1.00 99.44
jak,	ATOM	1399	CB	GLU A	182	-5.854	57.142	37.356	1.00 98.57
# *	ATOM	1400	CG	GLU A	182	-5.880	57.077	35.816	1.00100.00
1500 1500	ATOM	1401	CD	GLU A	182	-7.013	57.938	35.300	1.00100.00
25	ATOM	1402	OE1	GLU A	182	-7.817	58.385	36.105	1.00100.00
jest.	ATOM	1403	OE2	GLU A		-7.084	58.153	34.091	1.00100.00
	ATOM	1404	N	ASP A		-4.607	58.672	40.265	1.00 98.63
# # c	ATOM	1405	CA	ASP A		-5.021	59.257	41.552	1.00 97.49
	ATOM	1406	C	ASP A		-4.126	60.472	41.932	1.00100.00
1. 30	ATOM	1407	0	ASP A		-3.464	61.061	41.079	1.00100.00
1 2	ATOM	1408	CB	ASP A		-4.946	58.144	42.619	1.00 98.36
	ATOM	1409	CG	ASP A		-3.612	57.409	42.547	1.00100.00
197 II)	ATOM ATOM	1410 _. 1411		ASP A		-3.471	56.556	41.668	1.00100.00
₩ 35	ATOM	1412	N	ASP A PRO A		-2.741 -4.187	57.688 60.906	43.364 43.237	1.00100.00
	ATOM	1413	CA	PRO A		-3.311	61.985	43.738	1.00 97.96 1.00 97.92
	ATOM	1414	C	PRO A		-1.865	61.528	44.071	1.00 97.89
	ATOM	1415	Ö	PRO A		-1.348	61.748	45.159	1.00100.00
	ATOM	1416	CB	PRO A		-3.973	62.561	44.992	1.00 98.86
40	ATOM	1417	CG	PRO A		-5.262	61.777	45.284	1.00100.00
	ATOM	1418	CD	PRO A		-5.122	60.532	44.284	1.00 97.20
	ATOM	1419	N	SER A	185	-1.249	60.840	43.071	1.00 82.40
	ATOM	1420	CA	SER A		0.196	60.496	43.086	1.00 75.26
AE	ATOM	1421	C	SER A		0.748	60.563	41.623	1.00 71.84
45	ATOM	1422	0	SER A		-0.006	60.525	40.670	1.00 77.97
	ATOM	1423	CB	SER A		0.337	59.068	43.636	1.00 73.41
	ATOM	1424	OG	SER A		0.672	59.109	45.027	1.00 63.60
	ATOM	1425	N	ARG A		2.107	60.704	41.461	1.00 57.89
50	ATOM ATOM	1426 1427	CA C	ARG A		2.650	60.971	40.088	1.00 56.00
50	ATOM	1428	o	ARG A		3.725 4.473	59.943 60.157	39.633 38.688	1.00 59.64
	ATOM	1429	СВ	ARG A		3.258	62.393	40.064	1.00 60.30 1.00 63.74
	ATOM	1430	CG	ARG A		2.339	63.457	40.677	1.00 80.44
	ATOM	1431	CD	ARG A		1.188	63.874	39.736	1.00 71.31
55	ATOM	1432	NE	ARG A		1.316	63.215	38.436	1.00 79.64
	ATOM	1433	CZ	ARG A		0.185	62.862	37.784	1.00 95.30
	ATOM	1434		ARG A		-0.999	63.109	38.312	1.00 56.25
	ATOM	1435		ARG A		0.276	62.232	36.603	1.00 89.98
60	MOTA	1436	N	LYS A		3.892	58.778	40.265	1.00 54.50
60	ATOM	1437	CA	LYS A		4.891	57.805	39.851	1.00 51.93
	MOTA	1438	С	LYS A		4.506	56.436	40.276	1.00 52.96
	ATOM	1439	0	LYS A		3.971	56.236	41.368	1.00 53.58
	ATOM	1440	CB	LYS A		6.247	58.047	40.470	1.00 53.78
	MOTA	1441	CG	LYS A	187	7.427	57.714	39.574	1.00 43.05

	ATOM	1442	CD	LYS A	187	8.517	58.761	39.762	1.00 53.36
	ATOM	1443	CE	LYS A	187	9.870	58.468	39.146	1.00 39.68
•	ATOM	1444	NZ	LYS A		10.795	59.601	39.341	1.00 40.19
		1445		ILE A					
_	ATOM		N			4.819	55.502	39.403	1.00 46.36
5	ATOM	1446	CA	ILE A	188	4.565	54.128	39.700	1.00 43.57
	ATOM	1447	С	ILE A	188	5.824	53.311	39.851	1.00 42.64
	ATOM	1448	0	ILE A	188	6.647	53.189	38.937	1.00 41.55
			CB						
	MOTA	1449		ILE A		3.579	53.425	38.826	1.00 45.64
	MOTA	1450		ILE A	188	2.193	54.021	39.047	1.00 45.82
10	ATOM	1451	CG2	ILE A	188	3.590	51.969	39,273	1.00 43.43
	ATOM	1452	CDI	ILE A		1.448	53.505	40.276	1.00 62.08
	ATOM	1453	N	TYR A		5.950	52.757	41.042	1.00 35.58
	MOTA	1454	CA	TYR A		7.079	51.933	41.356	1.00 37.57
	ATOM	1455	С	TYR A	189	6.652	50.465	41.359	1.00 44.89
15	ATOM	1456	0	TYR A	189	5.656	50.092	41.999	1.00 44.33
	ATOM	1457	CB	TYR A					
						7.752	52.392	42.661	1.00 37.85
	MOTA	1458	CG	TYR A		8.692	53.563	42.456	1.00 34.49
C)	ATOM	1459	CD1	TYR A	189	9.968	53.375	41.930	1.00 35.93
19 = 10 ¹ 1 Jan	ATOM	1460	CD2	TYR A		8.310	54.859	42.813	1.00 32.44
1 20 i	ATOM	1461	CE1	TYR A					
13 ZV						10.843	54.449	41.753	1.00 36.88
1 :	ATOM	1462	CE2	TYR A		9.170	55.945	42.647	1.00 31.63
1.1.	MOTA	1463	CZ	TYR A		10.441	55.734	42.113	1.00 44.54
44 4 4	ATOM	1464	OH	TYR A	189	11.296	56.788	41.929	1.00 57.77
	ATOM	1465	N	LYS A		7.413			
75							49.651	40.608	1.00 42.91
<u>j</u> 25	ATOM	1466	CA	LYS A		7.173	48.210	40.420	1.00 42.22
J=4.	ATOM	1467	С	LYS A	190	8.152	47.262	41.143	1.00 40.73
	MOTA	1468	0	LYS A	190	9.398	47.400	41.093	1.00 35.69
#	MOTA	1469	СВ	LYS A		7.007	47.839	38.944	1.00 45.87
]=4x									
1677 14	ATOM	1470	CG	LYS A		5.735	48.403	38.306	1.00 71.08
30	ATOM	1471	CD	LYS A	190	5.758	48.384	36.779	1.00 84.62
n.	ATOM	1472	CE	LYS A	190	4.386	48.157	36.147	1.00100.00
	ATOM	1473	NZ	LYS A		4.299	46.930	35.329	1.00100.00
'ಗಿತ್ತಾದ್ದರೆ. 									
	ATOM	1474	N	PHE A		7.539	46.264	41.812	1.00 35.01
3_5	MOTA	1475	CA	PHE A	191	8.276	45.304	42.592	1.00 31.57
35	ATOM	1476	С	PHE A	191	7.792	43.871	42.465	1.00 30.89
	ATOM	1477	0	PHE A		6.603	43.584	42.377	1.00 25.06
	ATOM	1478	СВ	PHE A					
						8.217	45.734	44.080	1.00 32.11
	ATOM	1479	CG	PHE A		8.570	47.190	44.372	1.00 29.24
	ATOM	1480		PHE A		9.895	47.593	44.539	1.00 31.81
40	ATOM	1481	CD2	PHE A	191	7.565	48.147	44.508	1.00 30.17
	MOTA	1482		PHE A		10.230	48.925	44.805	1.00 34.10
		1483		PHE A					
	ATOM					7.866	49.483	44.776	1.00 33.69
	MOTA	1484	CZ	PHE A	191	9.201	49.860	44.928	1.00 33.32
	ATOM	1485	N	ILE A	192	8.764	42.961	42.505	1.00 35.75
45	MOTA	1486	CA	ILE A	192	8.525	41.520	42.415	1.00 37.02
	MOTA	1487	C	ILE A		9.255	40.653		
								43.469	1.00 33.05
	ATOM	1488	0	ILE A		10.489	40.672	43.593	1.00 30.73
	ATOM	1489	CB	ILE A	192	8.850	40.970	41.025	1.00 42.45
	ATOM	1490	CG1	ILE A	192	8.289	41.914	39.981	1.00 46.39
50	MOTA	1491		ILE A		8.251	39.567	40.859	1.00 44.02
	ATOM	1492		ILE A					
						7.609	41.231	38.798	1.00 69.61
	MOTA	1493	N	GLN A		8.459	39.864	44.195	1.00 27.51
	ATOM	1494	CA	GLN A	193	8.954	38.908	45.177	1.00 32.05
	MOTA	1495	С	GLN A	193	8.626	37.488	44.757	1.00 44.32
55	ATOM	1496	ō						
				GLN A		7.583	36.926	45.120	1.00 43.11
	ATOM	1497	CB	GLN A		8.502	39.100	46.638	1.00 33.44
	ATOM	1498	CG	GLN A	193	9.285	38.203	47.632	1.00 22.34
	ATOM	1499	CD	GLN A		10.824	38.337	47.636	1.00 48.52
	ATOM	1500	OE1						
4 0						11.557	37.537	47.016	1.00 45.24
60	ATOM	1501	NE2			11.326	39.330	48.373	1.00 24.82
	ATOM	1502	N	LYS A	194	9.543	36.908	43.993	1.00 46.91
	ATOM	1503	CA	LYS A		9.384	35.540	43.529	1.00 47.56
	ATOM	1504	С	LYS A		9.456	34.524	44.666	1.00 49.56
	ATOM	1505	ŏ						
	ATOM	1202	•	LYS A	174	8.777	33.520	44.598	1.00 50.85

35.159 MOTA 1506 CB LYS A 194 10.385 42.439 1.00 48.11 LYS A 194 9.884 ATOM 1507 CG 35.443 41.031 1.00 55.70 10.895 MOTA 1508 CD LYS A 194 36.200 40.179 1.00 67.67 1509 CE LYS A 194 10.614 36.122 38.682 MOTA 1.00 81.92 5 1510 LYS A 194 11.284 37.185 37.910 ATOM NZ 1.00 88.34 34.753 33.780 ATOM 1511 N VAL A 195 10.308 45.689 1.00 39.55 46.764 VAL A 195 ATOM 1512 CA 10.422 1.00 33.56 33.862 1513 VAL A 195 9.261 47.698 1.00 35.67 С MOTA 1.00 38.69 VAL A 195 8.804 34.945 MOTA 1514 0 48.034 10 ATOM 1515 CB VAL A 195 11.716 33.844 47.560 1.00 32.62 1516 CG1 VAL A 195 11.849 32.539 48.310 ATOM 1.00 32.40 1517 CG2 VAL A 195 12.933 34.029 46.667 ATOM 1.00 30.55 PRO A 196 8.770 32.717 48.126 ATOM . 1518 N 1.00 27.75 ATOM 1519 CA PRO A 196 7.653 32.757 49.038 1.00 26.18 15 33.236 PRO A 196 8.132 ATOM 1520 С 50.410 1.00 35.86 1521 PRO A 196 9.185 32.809 ATOM 0 50.899 1.00 35.43 1522 CB PRO A 196 7.022 31.359 49.044 1.00 26.04 ATOM MOTA 1523 PRO A 196 7.856 30.472 1.00 27.79 CG 48.113 1524 CD PRO A 196 8.964 31.352 47.546 MOTA 1.00 25.40 20 1525 ILE A 197 7.388 34.171 MOTA N 51.009 1.00 29.92 1526 ILE A 197 7.772 CA 34.697 ATOM 52.284 1.00 26.98 4 1527 С ILE A 197 6.544 34.809 53.128 ATOM 1.00 34.88 1528 ILE A 197 5.444 34.788 52.606 ATOM 0 1.00 29.68 ATOM 1529 CB ILE A 197 8.334 36.100 52.094 1.00 27.90 1.00 27.78 1.00 28.12 1.00 19.03 CG1 ILE A 197 51.254 51.337 1530 **ATOM** 7.342 36.867 1531 CG2 ILE A 197 36.091 ATOM 9.659 1532 CD1 ILE A 197 7.494 38.378 51.438 ATOM h-i 1.00 36.02 MOTA 1533 N PRO A 198 6.743 34.936 54.447 5.647 ATOM 1534 CA PRO A 198 35.110 55.410 1.00 31.31 30 PRO A 198 1535 5.299 MOTA С 36.583 55.308 1.00 28.27 PRO A 198 1536 6.212 37.391 55.115 ATOM 0 1.00 22.70 6.252 ATOM 1537 CB PRO A 198 34.849 56.794 1.00 31.17 1 ATOM 1538 CG PRO A 198 7.768 34.768 56.615 1.00 34.94 PRO A 198 34.706 1539 CD 8.057 55.122 1.00 32.99 ATOM 35 ATOM 1540 CYS A 199 4.011 36.939 55.405 N 1.00 27.60 3.555 1541 CYS A 199 38.360 **ATOM** CA 55.289 1.00 27.66 ATOM 1542 С CYS A 199 4.255 39.390 56.187 1.00 30.13 ATOM 1543 0 CYS A 199 4.294 40.596 55.895 1.00 29.50 1544 CB CYS A 199 38.534 ATOM 2.025 55.242 1.00 27.18 40 1545 CYS A 199 56.841 1.00 30.85 ATOM SG 1.232 38.279 TYR A 200 1.00 26.15 ATOM 1546 N 4.847 38.903 57.270 TYR A 200 58.123 57.483 1.00 28.28 1.00 32.29 1547 5.538 39.798 ATOM CA 1548 TYR A 200 6.760 40.395 ATOM С TYR A 200 1549 7.359 41.286 1.00 31.56 ATOM 0 58.036 45 1.00 30.59 1550 **TYR A 200** 5.844 39.215 ATOM CB 59.489 MOTA 1551 CG TYR A 200 6.989 38.272 59.568 1.00 28.28 CD1 TYR A 200 MOTA 1552 8.288 38.733 59.689 1.00 29.48 6.756 1553 CD2 TYR A 200 36.903 59.475 MOTA 1.00 27.55 CE1 TYR A 200 9.377 37.862 ATOM 1554 59.825 1.00 21.42 50 TYR A 200 ATOM 1555 CE2 7.838 36.015 59.595 1.00 27.41 TYR A 200 **ATOM** 1556 9.144 59.737 CZ36.488 1.00 25.11 ATOM 1557 TYR A 200 10.215 35.614 59.880 OH 1.00 27.62 1558 LEU A 201 7.113 ATOM 39.897 56.313 N 1.00 31.66 ATOM 1559 CA **LEU A 201** 8.278 40.378 55.579 1.00 29.49 55 1560 LEU A 201 7.914 MOTA С 41.343 54.484 1.00 33.65 LEU A 201 8.767 MOTA 1561 41.737 0 53.686 1.00 35.31 LEU A 201 MOTA 1562 CB 9.225 39.275 55.035 1.00 27.04 MOTA 1563 CG LEU A 201 9.697 38.271 56.071 1.00 27.42 LEU A 201 ATOM 1564 CD1 10.254 37.030 55.390 1.00 23.71 60 1565 CD2 LEU A 201 10.764 1.00 30.55 **ATOM** 38.913 56.957 ILE A 202 1.00 28.66 ATOM 1566 N 6.648 41.710 54.438 ATOM 1567 ILE A 202 6.249 CA 42.674 53.433 1.00 29.57 ATOM 1568 C ILE A 202 6.636 44.074 53.951 1.00 40.28 6.192 ILE A 202 ATOM 1569 0 44.493 55.027 1.00 40.75

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ATOM 1571 CC2 LILE À 202		MOTA	1570	СВ	ILE A	202	4.733	42.651	53.182	1.00 31.18
TOM 1572 CG2 ILE A 202 4.259 43.962 52.521 1.00 29.23 ATOM 1574 N ALA A 203 7.445 44.813 53.197 1.00 39.14 ATOM 1575 CA ALA A 203 7.840 46.150 53.611 1.00 37.03 ATOM 1576 CA ALA A 203 7.840 46.150 53.611 1.00 37.03 ATOM 1576 CA ALA A 203 7.849 47.159 52.482 1.00 34.32 ATOM 1577 O ALA A 203 9.180 46.143 54.309 1.00 38.22 ATOM 1578 N EU A 204 7.514 48.388 52.910 1.00 38.22 ATOM 1580 CA LEU A 204 7.514 48.388 52.910 1.00 38.22 ATOM 1580 CA LEU A 204 7.888 49.604 52.102 1.00 32.56 ATOM 1581 C LEU A 204 7.893 50.817 52.812 1.00 37.03 ATOM 1582 C LEU A 204 7.894 9.929 51.718 1.00 29.74 ATOM 1586 CD LEU A 204 7.894 50.817 52.812 1.00 37.03 ATOM 1586 CD LEU A 204 7.894 50.817 52.812 1.00 37.03 ATOM 1586 CD LEU A 204 7.894 50.817 52.812 1.00 37.03 ATOM 1586 CD LEU A 204 7.894 50.817 52.812 1.00 37.03 ATOM 1586 CD LEU A 204 7.894 50.817 52.812 1.00 37.03 ATOM 1588 CA VAL A 205 9.96 49.929 51.718 1.00 29.74 ATOM 1588 CA VAL A 205 9.305 52.821 52.415 1.00 38.50 ATOM 1589 C VAL A 205 9.305 52.821 52.415 1.00 38.50 ATOM 1580 C VAL A 205 9.305 52.821 52.415 1.00 38.50 ATOM 1590 C VAL A 205 9.575 53.462 50.148 1.00 38.50 ATOM 1590 C VAL A 205 9.575 53.462 50.148 1.00 39.50 ATOM 1590 C VAL A 205 9.575 53.462 50.148 1.00 38.50 ATOM 1590 C VAL A 205 9.575 53.462 50.148 1.00 38.50 ATOM 1590 C VAL A 205 9.575 53.462 50.148 1.00 38.50 ATOM 1590 C VAL A 205 9.575 53.462 50.148 1.00 38.50 ATOM 1590 C VAL A 206 8.623 56.104 50.687 1.00 31.98 ATOM 1590 C VAL A 206 8.623 56.104 50.687 1.00 31.98 ATOM 1590 C VAL A 206 8.623 56.104 50.687 1.00 31.98 ATOM 1590 C VAL A 206 9.076 57.722 52.406 1.00 33.54 ATOM 1590 C VAL A 206 9.076 57.722 52.406 1.00 34.81 ATOM 1590 C VAL A 206 9.076 57.722 52.406 1.00 34.81 ATOM 1590 C VAL A 206 9.076 57.723 50.433 1.00 42.72 ATOM 1600 N GLY A 207 11.00 75.95 50.431 1.00 40.93 ATOM 1600 N LEU A 209 14.620 59.97 49.987 1.00 51.00 ATOM 1600 N LEU A 209 14.620 59.97 49.987 1.00 51.00 ATOM 1600 N LEU A 209 14.620 59.97 49.987 1.00 31.48 ATOM 1600 N LEU A 209 14.620 59.97 49.										
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10 ATOM 1578 CB ALA 203 8.060 46.836 51.311 1.00 30.63 1.00 ATOM 1579 N LEU A 204 7.514 48.388 52.910 1.00 38.22 ATOM 1580 CA LEU A 204 7.386 49.604 52.102 1.00 37.69 ATOM 1581 C LEU A 204 7.386 49.604 52.102 1.00 37.69 ATOM 1581 C LEU A 204 7.935 50.817 54.034 1.00 37.69 ATOM 1583 CB LEU A 204 7.836 19.037 54.034 1.00 32.66 ATOM 1583 CB LEU A 204 5.906 49.929 51.718 1.00 29.74 ATOM 1586 CD LEU A 204 5.906 49.929 51.718 1.00 29.74 ATOM 1586 CD LEU A 204 5.706 51.182 50.855 1.00 29.47 ATOM 1587 N VAL A 205 8.670 51.082 50.994 49.45 1.00 36.67 ATOM 1588 CA VAL A 205 9.305 52.821 52.415 1.00 36.87 ATOM 1589 C VAL A 205 9.305 52.821 52.415 1.00 36.87 ATOM 1590 C VAL A 205 9.224 53.795 51.684 1.00 38.41 ATOM 1591 CB VAL A 205 9.525 52.651 52.804 1.00 38.41 ATOM 1591 CB VAL A 205 9.525 52.651 52.804 1.00 38.41 ATOM 1591 CB VAL A 205 9.525 52.651 52.804 1.00 36.66 ATOM 1593 CG2 VAL A 205 9.575 53.462 50.148 1.00 35.58 ATOM 1593 CG2 VAL A 205 11.432 54.020 52.651 52.804 1.00 35.58 ATOM 1595 CG2 VAL A 205 11.442 54.020 52.651 52.804 1.00 35.98 ATOM 1595 CG2 VAL A 206 8.623 56.104 51.757 1.00 35.08 ATOM 1595 CG2 VAL A 206 8.623 56.104 50.687 1.00 31.81 ATOM 1595 CG2 VAL A 206 8.623 56.104 50.687 1.00 31.54 ATOM 1599 CG2 VAL A 206 8.623 56.104 50.687 1.00 31.81 ATOM 1596 C VAL A 206 9.006 57.722 52.406 1.00 34.81 ATOM 1590 CG2 VAL A 206 9.006 57.722 52.406 1.00 33.35 ATOM 1599 CG1 VAL A 206 9.006 57.722 52.406 1.00 33.35 ATOM 1590 CG2 VAL A 206 9.300 57.543 51.623 1.00 33.35 ATOM 1500 CG2 VAL A 206 9.300 57.543 51.623 1.00 33.35 ATOM 1500 CG2 VAL A 206 9.300 57.543 51.623 1.00 33.35 ATOM 1500 CG2 VAL A 206 9.300 57.543 51.623 1.00 33.35 ATOM 1500 CG2 VAL A 206 9.300 57.543 51.623 1.00 33.35 ATOM 1500 CG2 VAL A 206 9.300 57.543 51.623 1.00 33.35 ATOM 1500 CG2 VAL A 206 9.300 57.543 51.49 1.00 33.35 ATOM 1500 CG2 VAL A 206 9.306 57.722 52.406 1.00 34.81 ATOM 1500 CG2 VAL A 206 9.306 57.723 50.49 49.929 1.00 33.44 ATOM 1500 CG2 VAL A 206 9.306 57.543 49.929 1.00 33.45 ATOM 1500 CG2 VAL A 206 9.306 57.543 49.929 1.00 33.45 AT										1.00 37.03
10 ATOM 1578 CB ALA A 203 9,180 46,143 54,309 1.00 33,64 ATOM 1580 CA LEU A 204 7,514 48,388 52,910 1.00 33,64 ATOM 1581 C LEU A 204 7,538 49,604 52,102 1.00 32,66 ATOM 1582 O LEU A 204 7,938 49,604 52,102 1.00 32,66 ATOM 1582 O LEU A 204 7,938 50,817 52,812 1.00 37,69 ATOM 1582 O LEU A 204 5,906 49,929 51,718 1.00 29,64 ATOM 1585 CB LEU A 204 5,706 51,102 50,855 1.00 29,64 ATOM 1586 CD LEU A 204 6,263 50,994 49,445 1.00 29,64 ATOM 1586 CD LEU A 204 6,263 50,994 49,445 1.00 29,47 ATOM 1586 CD LEU A 204 4,222 51,515 50,750 1.00 33,50 ATOM 1588 CA VAL A 205 8,670 51,603 51,991 1.00 36,515 ATOM 1589 C VAL A 205 9,305 52,821 52,415 1.00 35,15 ATOM 1589 C VAL A 205 9,305 52,821 52,415 1.00 39,50 ATOM 1589 C VAL A 205 9,575 53,462 50,148 1.00 38,41 ATOM 1591 CB VAL A 205 10,769 52,651 52,804 1.00 38,41 ATOM 1592 CGI VAL A 205 11,466 51,794 51,757 1.00 35,08 ATOM 1593 CG2 VAL A 205 11,466 51,794 51,757 1.00 35,08 ATOM 1593 CG2 VAL A 205 11,466 51,794 51,757 1.00 35,08 ATOM 1595 CGI VAL A 205 11,466 51,794 51,757 1.00 35,08 ATOM 1595 CGI VAL A 205 11,462 51,402 52,833 1.00 35,94 ATOM 1595 CGI VAL A 205 11,462 51,402 52,833 1.00 33,84 ATOM 1595 CGI VAL A 206 8,750 54,983 51,623 1.00 33,84 ATOM 1595 CGI VAL A 206 8,750 54,983 51,623 1.00 33,84 ATOM 1595 CGI VAL A 206 9,300 57,343 51,249 1.00 31,84 ATOM 1595 CGI VAL A 206 9,300 57,343 51,249 1.00 31,84 ATOM 1595 CGI VAL A 206 9,300 57,343 51,249 1.00 31,84 ATOM 1595 CGI VAL A 206 9,300 57,343 51,249 1.00 31,84 ATOM 1595 CGI VAL A 206 9,300 57,343 51,249 1.00 31,94 ATOM 1595 CGI VAL A 206 9,300 57,343 51,249 1.00 31,94 ATOM 1590 CGI VAL A 206 9,300 57,343 51,249 1.00 31,94 ATOM 1500 CGI VAL A 206 9,300 57,343 51,249 1.00 31,94 ATOM 1500 CGI VAL A 206 9,300 57,343 51,249 1.00 31,94 ATOM 1500 CGI VAL A 206 9,300 57,343 51,249 1.00 31,94 ATOM 1500 CGI VAL A 206 9,305 51,305 51,300 31,34 ATOM 1500 CGI VAL A 206 9,305 51,305 51,305 51,300 31,300 31,34 ATOM 1500 CGI VAL A 206 9,305 51,305 51,305 51,300 31,300 31,34 ATOM 1500 CGI VAL A 206 9,305 51,305 51,305 51,300 31,300 31,30		MOTA		С			7.819	47.159		1.00 34.32
10 ATOM 1579 N LEU A 204 7.384 48.388 52.910 1.00 33.64 ATOM 1581 C LEU A 204 7.383 49.604 52.102 1.00 32.56 ATOM 1581 C LEU A 204 7.884 49.604 52.102 1.00 32.56 ATOM 1582 O LEU A 204 7.884 51.037 54.034 1.00 32.66 ATOM 1583 CB LEU A 204 5.906 49.929 51.718 1.00 29.74 ATOM 1585 CD LEU A 204 5.906 49.929 51.718 1.00 29.74 ATOM 1585 CD LEU A 204 6.263 50.994 49.445 1.00 32.56 ATOM 1587 N VAL A 205 50.905 51.603 51.991 1.00 36.87 ATOM 1589 C VAL A 205 9.305 52.821 52.415 1.00 36.87 ATOM 1589 C VAL A 205 9.305 52.821 52.415 1.00 36.87 ATOM 1589 C VAL A 205 9.254 53.795 51.284 1.00 38.41 ATOM 1591 CB VAL A 205 9.575 53.462 50.148 1.00 38.41 ATOM 1591 CB VAL A 205 9.575 53.462 50.148 1.00 36.06 ATOM 1593 CGZ VAL A 205 10.769 52.651 52.804 1.00 36.06 ATOM 1593 CGZ VAL A 205 11.432 54.020 52.833 1.00 35.98 ATOM 1593 CGZ VAL A 205 11.432 54.020 52.833 1.00 35.98 ATOM 1595 CG VAL A 205 11.436 51.794 51.757 1.00 35.98 ATOM 1595 CG VAL A 206 8.623 56.104 50.687 1.00 35.98 ATOM 1595 CGZ VAL A 206 8.623 56.104 50.687 1.00 31.62 ATOM 1596 C VAL A 206 8.623 56.104 50.687 1.00 31.62 ATOM 1596 C VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1596 C VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1598 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1598 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1598 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1598 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1598 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1598 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1598 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1598 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1598 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1598 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1500 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.98 ATOM 1500 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1500 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1500 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.98 ATOM 1500 CGZ VAL A 206 9.300 57.343 51.249 1.00 31.98 ATOM 1500 CGZ VAL A 206 9.300 5		ATOM	1577	0	ALA A	203	8.060	46.836	51.311	1.00 30.63
10 ATOM 1579 N LEU A 204 7.384 48.388 52.910 1.00 33.64 ATOM 1581 C LEU A 204 7.389 49.604 52.102 1.00 32.56 ATOM 1582 O LEU A 204 7.884 51.037 54.034 1.00 32.66 ATOM 1583 CB LEU A 204 7.884 51.037 54.034 1.00 32.66 ATOM 1583 CB LEU A 204 5.706 49.929 51.718 1.00 29.74 ATOM 1585 CD1 LEU A 204 6.263 50.994 49.445 1.00 29.74 ATOM 1585 CD1 LEU A 204 6.263 50.994 49.445 1.00 29.47 ATOM 1586 CD2 LEU A 204 6.263 50.994 49.445 1.00 29.47 ATOM 1586 CD2 LEU A 204 4.222 51.515 50.750 1.00 33.687 ATOM 1587 N VAL A 205 9.305 52.821 52.415 1.00 36.87 ATOM 1589 C VAL A 205 9.305 52.821 52.415 1.00 35.15 ATOM 1589 C VAL A 205 9.254 53.795 51.284 1.00 36.06 ATOM 1591 CB VAL A 205 9.575 53.462 50.148 1.00 36.06 ATOM 1591 CB VAL A 205 10.769 52.651 52.804 1.00 36.06 ATOM 1591 CB VAL A 205 10.769 52.651 52.804 1.00 36.96 ATOM 1593 CG2 VAL A 205 11.466 51.794 51.757 1.00 35.98 ATOM 1593 CG2 VAL A 205 11.466 51.794 51.757 1.00 35.98 ATOM 1595 CA VAL A 206 8.623 56.104 50.687 1.00 31.81 ATOM 1595 CA VAL A 206 8.623 56.104 50.687 1.00 31.81 ATOM 1595 CA VAL A 206 8.623 56.104 50.687 1.00 31.81 ATOM 1595 CA VAL A 206 8.623 56.104 50.687 1.00 31.81 ATOM 1598 CB VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1598 CB VAL A 206 7.179 56.405 50.305 1.00 33.35 ATOM 1598 CB VAL A 206 7.129 57.223 49.029 1.00 31.81 ATOM 1598 CB VAL A 206 7.129 57.223 49.029 1.00 31.82 ATOM 1598 CB VAL A 206 7.129 57.223 49.029 1.00 31.82 ATOM 1598 CB VAL A 206 7.129 57.243 49.029 1.00 31.82 ATOM 1598 CB VAL A 206 7.129 57.243 49.029 1.00 31.82 ATOM 1598 CB VAL A 206 7.129 57.243 49.029 1.00 31.82 ATOM 1598 CB VAL A 206 7.129 57.243 49.029 1.00 31.82 ATOM 1598 CB VAL A 206 7.129 57.243 49.029 1.00 31.82 ATOM 1598 CB VAL A 208 11.429 55.045 50.085 1.00 39.98 ATOM 1501 CC2 VAL A 206 7.129 57.243 49.029 1.00 31.82 ATOM 1508 CC VAL A 208 11.429 50.085 50.851 1.00 39.98 ATOM 1501 CC2 VAL A 208 11.429 50.833 50.129 1.00 31.98 ATOM 1501 CC2 VAL A 208 11.429 50.833 50.129 1.00 31.98 ATOM 1501 CC2 VAL A 208 11.30 50.833 50.129 1.00 31.98 ATOM 1501 CC2 VAL A 208 11.30 5		MOTA	1578	CB	ALA A	203	9.180	46.143	54.309	
ATOM 1580 CA LEU A 204 7.993 50.817 52.812 1.00 37.69 ATOM 1582 O LEU A 204 7.993 50.817 52.812 1.00 37.69 ATOM 1583 CB LEU A 204 7.993 50.817 52.812 1.00 37.69 ATOM 1584 CG LEU A 204 5.906 49.929 51.718 1.00 29.74 ATOM 1586 CD LEU A 204 6.263 50.994 49.445 1.00 29.74 ATOM 1586 CD LEU A 204 6.263 50.994 49.445 1.00 29.47 ATOM 1586 CD LEU A 204 6.263 50.994 49.445 1.00 29.47 ATOM 1588 CA VAL A 205 8.670 51.603 51.991 1.00 36.87 ATOM 1588 CA VAL A 205 9.305 52.821 52.415 1.00 35.15 ATOM 1589 C VAL A 205 9.305 52.821 52.415 1.00 35.15 ATOM 1589 C VAL A 205 9.524 53.795 51.284 1.00 39.50 ATOM 1589 C VAL A 205 9.575 53.462 50.148 1.00 39.50 ATOM 1591 CB VAL A 205 10.769 52.651 52.804 1.00 36.87 ATOM 1592 CGI VAL A 205 11.466 51.794 51.757 1.00 35.08 ATOM 1593 CG2 VAL A 205 11.466 51.794 51.757 1.00 35.08 ATOM 1595 CA VAL A 205 11.465 51.794 51.757 1.00 35.08 ATOM 1595 CA VAL A 206 8.623 56.104 50.687 1.00 35.08 ATOM 1595 CA VAL A 206 8.623 56.104 50.687 1.00 31.81 ATOM 1595 CA VAL A 206 9.076 57.722 52.406 1.00 33.451 ATOM 1599 CGI VAL A 206 9.076 57.722 52.406 1.00 33.451 ATOM 1599 CGI VAL A 206 7.129 57.243 49.029 1.00 31.63 ATOM 1599 CGI VAL A 206 7.129 57.243 49.029 1.00 31.63 ATOM 1599 CGI VAL A 206 7.129 57.243 49.029 1.00 31.63 ATOM 1600 CG2 VAL A 206 7.129 57.243 49.029 1.00 31.63 ATOM 1600 CG2 VAL A 206 7.129 57.243 49.029 1.00 31.63 ATOM 1600 CG2 VAL A 206 7.129 57.243 49.029 1.00 31.63 ATOM 1606 CA ALA A 208 13.370 61.354 49.293 1.00 42.94 ATOM 1606 CA ALA A 208 13.370 61.354 49.293 1.00 42.94 ATOM 1606 CC ALA A 208 13.370 61.354 49.293 1.00 42.94 ATOM 1606 CC ALA A 208 13.300 57.93 50.431 1.00 42.94 ATOM 1606 CC ALA A 208 13.300 57.93 50.431 1.00 42.94 ATOM 1606 CC ALA A 208 13.300 57.93 50.431 1.00 42.94 ATOM 1607 C ALA A 208 13.300 57.93 50.431 1.00 42.94 ATOM 1608 C ALA A 208 13.300 57.93 50.431 1.00 42.94 ATOM 1608 C ALA A 208 13.605 68.803 50.129 1.00 40.46 ATOM 1601 C BLU A 209 16.456 58.966 48.840 1.00 47.95 ATOM 1601 C BLU A 209 16.456 58.966 48.840 1.00 43.31	10	MOTA	1579	N	LEU A	204	7.514	48.388		
ATOM 1581 C LEU A 204 7.893 50.817 52.812 1.00 37.69 ATOM 1582 O LEU A 204 7.894 51.037 54.034 1.00 32.66 ATOM 1583 CB LEU A 204 5.906 49.929 51.718 1.00 29.74 ATOM 1585 CD LEU A 204 5.706 51.162 50.855 1.00 29.47 ATOM 1586 CD LEU A 204 6.263 50.994 49.445 1.00 29.47 ATOM 1587 N VAL A 205 8.670 51.603 51.991 1.00 36.87 ATOM 1589 C AL A 205 9.305 52.821 52.415 1.00 38.61 ATOM 1589 C AL A 205 9.305 52.821 52.415 1.00 38.41 ATOM 1591 CB VAL A 205 9.575 53.462 50.148 1.00 39.50 ATOM 1591 CB VAL A 205 9.575 53.462 50.148 1.00 39.50 ATOM 1591 CB VAL A 205 10.769 52.651 52.804 1.00 38.60 ATOM 1594 N VAL A 205 11.466 51.794 51.757 1.00 35.08 ATOM 1595 CA VAL A 205 11.466 51.794 51.757 1.00 35.08 ATOM 1595 CA VAL A 205 11.466 51.794 51.603 1.00 33.54 ATOM 1595 CA VAL A 206 8.623 56.104 50.667 1.00 31.81 ATOM 1595 CA VAL A 206 9.300 57.343 51.249 1.00 33.54 ATOM 1595 CA VAL A 206 9.300 57.343 51.249 1.00 33.54 ATOM 1595 CA VAL A 206 9.300 57.343 51.249 1.00 33.54 ATOM 1595 CA VAL A 206 9.300 57.343 51.249 1.00 33.54 ATOM 1595 CA VAL A 206 9.300 57.343 51.249 1.00 33.54 ATOM 1595 CA VAL A 206 9.300 57.343 51.249 1.00 33.54 ATOM 1595 CA VAL A 206 9.300 57.343 51.249 1.00 33.45 ATOM 1500 CG2 VAL A 206 7.179 56.405 50.305 1.00 33.55 ATOM 1500 CG2 VAL A 206 7.179 56.405 50.305 1.00 33.55 ATOM 1601 N GLY A 207 10.180 57.995 50.431 1.00 27.25 ATOM 1602 CA GLY A 207 10.807 59.168 50.861 1.00 27.25 ATOM 1605 N ALA 208 13.370 61.354 49.233 1.00 42.92 ATOM 1606 CA ALA 208 13.370 61.354 49.233 1.00 42.92 ATOM 1607 C ALA 208 13.370 61.354 49.233 1.00 42.92 ATOM 1608 C ALA 208 13.605 62.810 49.589 1.00 43.93 ATOM 1609 CB ALA 208 13.605 62.810 49.589 1.00 43.93 ATOM 1601 N GLY A 207 11.802 59.635 48.873 1.00 47.96 ATOM 1611 CA EUU A 209 15.265 56.954 48.894 1.00 47.96 ATOM 1612 C C EUU A 209 15.265 56.954 48.894 1.00 47.95 ATOM 1610 N GLU A 200 15.265 60.91 50.103 1.00 40.90 ATOM 1611 CA EUU A 209 15.265 60.91 50.103 1.00 40.90 ATOM 1612 C C EUU A 209 15.265 60.91 50.005 1.00 40.90 ATOM 1613 O GER A		MOTA	1580	CA	LEU A	204				
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15 ATOM 1588 CB LEU A 204 5.906 49.929 51.718 1.00 29.74 ATOM 1585 CD1 LEU A 204 6.263 50.994 49.445 1.00 29.47 ATOM 1586 CD2 LEU A 204 4.222 51.515 50.750 1.00 33.50 ATOM 1587 N VAL A 205 8.670 51.603 51.991 1.00 36.87 N ATOM 1589 C VAL A 205 9.205 52.821 52.415 1.00 35.15 ATOM 1589 C VAL A 205 9.205 52.821 52.415 1.00 35.15 ATOM 1590 O VAL A 205 9.205 53.462 50.148 1.00 38.41 ATOM 1591 CB VAL A 205 9.575 53.462 50.148 1.00 38.41 ATOM 1591 CB VAL A 205 10.769 52.651 52.804 1.00 36.076 ATOM 1592 CG1 VAL A 205 11.466 51.794 51.757 1.00 35.08 ATOM 1593 CA VAL A 205 11.466 51.794 51.757 1.00 35.08 ATOM 1595 CA VAL A 206 8.750 54.983 51.623 1.00 33.54 ATOM 1595 CA VAL A 206 8.750 54.983 51.623 1.00 33.54 ATOM 1595 CA VAL A 206 8.623 56.104 50.687 1.00 31.81 ATOM 1595 CA VAL A 206 9.300 57.343 51.249 1.00 31.62 ATOM 1596 CB VAL A 206 7.179 56.405 50.305 1.00 33.44 ATOM 1595 CB VAL A 206 7.179 56.405 50.305 1.00 33.44 ATOM 1596 CB VAL A 206 7.129 57.243 49.029 1.00 33.44 ATOM 1596 CB VAL A 206 7.129 57.243 49.029 1.00 33.44 ATOM 1509 CG1 VAL A 206 7.129 57.243 49.029 1.00 33.44 ATOM 1600 CG2 VAL A 206 6.452 55.084 50.109 1.00 33.44 ATOM 1601 N GLY A 207 10.130 57.959 50.431 1.00 24.94 ATOM 1603 C GLY A 207 10.807 59.168 50.861 1.00 27.25 ATOM 1603 C GLY A 207 10.807 59.168 50.861 1.00 27.25 ATOM 1603 C GLY A 207 10.807 59.168 50.861 1.00 27.25 ATOM 1609 CB ALA A 208 12.375 60.783 50.113 1.00 41.77 ATOM 1608 O ALA A 208 13.370 61.354 49.233 1.00 42.72 ATOM 1601 CA LEU A 209 14.623 59.350 48.773 1.00 40.952 ATOM 1610 CC LEU A 209 14.623 59.350 48.773 1.00 40.952 ATOM 1611 CA LEU A 209 15.269 56.994 48.894 1.00 37.95 50.400 1611 CA LEU A 209 15.269 56.994 48.894 1.00 37.95 50.400 1611 CA LEU A 209 15.269 56.994 48.894 1.00 37.95 50.400 1611 CA LEU A 209 15.269 56.994 48.894 1.00 37.95 50.400 1611 CA LEU A 209 15.269 56.994 48.894 1.00 37.95 50.400 1611 CA LEU A 209 15.269 56.994 48.894 1.00 37.95 50.400 1611 CA LEU A 209 15.269 56.994 48.894 1.00 37.95 50.400 1611 CA LEU A 209 15.269 56.994 48.894 1.00 37.95 50.400 1611										
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ATOM 1603 C GLY A 207 11.802 59.632 49.838 1.00 38.81 ATOM 1605 N ALA A 208 12.375 60.783 50.113 1.00 41.07 ATOM 1606 CA ALA A 208 12.375 60.783 50.113 1.00 42.72 ATOM 1607 C ALA A 208 15.651 60.997 49.957 1.00 51.30 40.07 ATOM 1608 O ALA A 208 15.651 60.997 49.957 1.00 51.30 ATOM 1609 CB ALA A 208 13.605 62.810 49.589 1.00 42.95 ATOM 1610 N LEU A 209 14.623 59.350 48.773 1.00 40.92 ATOM 1611 CA LEU A 209 16.756 58.843 46.597 1.00 49.54 45 ATOM 1612 C LEU A 209 16.756 58.843 46.597 1.00 49.44 45 ATOM 1614 CB LEU A 209 15.269 56.994 48.894 1.00 37.97 ATOM 1615 CG LEU A 209 15.269 56.994 48.894 1.00 37.97 ATOM 1616 CD1 LEU A 209 15.269 56.994 48.894 1.00 37.97 ATOM 1616 CD1 LEU A 209 13.713 55.469 50.075 1.00 40.46 ATOM 1618 N GLU A 210 19.905 58.317 48.182 1.00 42.68 ATOM 1620 C GLU A 210 19.905 58.311 47.381 1.00 40.30 ATOM 1620 C GLU A 210 19.905 58.311 47.381 1.00 40.30 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.89 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 1.00 47.89 ATOM 1622 CB GLU A 210 19.905 57.056 47.6093 1.00 47.51 1.00 47.89 ATOM 1622 CB GLU A 210 20.884 59.553 47.613 1.00 42.01 ATOM 1622 CB GLU A 210 20.884 59.553 47.613 1.00 42.01 ATOM 1625 OGE GLU A 210 20.885 56.493 46.667 1.00 43.37 ATOM 1620 CD GER A 211 20.085 56.493	n.	ATOM	1601	N	GLY A	. 207	10.130		50.431	1.00 24.94
ATOM 1603 C GLY A 207 11.802 59.632 49.838 1.00 38.81 ATOM 1605 N ALA A 208 12.375 60.783 50.113 1.00 41.07 ATOM 1606 CA ALA A 208 12.375 60.783 50.113 1.00 42.72 ATOM 1607 C ALA A 208 15.651 60.997 49.957 1.00 51.30 40.07 ATOM 1608 O ALA A 208 15.651 60.997 49.957 1.00 51.30 ATOM 1609 CB ALA A 208 13.605 62.810 49.589 1.00 42.95 ATOM 1610 N LEU A 209 14.623 59.350 48.773 1.00 40.92 ATOM 1611 CA LEU A 209 16.756 58.843 46.597 1.00 49.54 45 ATOM 1612 C LEU A 209 16.756 58.843 46.597 1.00 49.44 45 ATOM 1614 CB LEU A 209 15.269 56.994 48.894 1.00 37.97 ATOM 1615 CG LEU A 209 15.269 56.994 48.894 1.00 37.97 ATOM 1616 CD1 LEU A 209 15.269 56.994 48.894 1.00 37.97 ATOM 1616 CD1 LEU A 209 13.713 55.469 50.075 1.00 40.46 ATOM 1618 N GLU A 210 19.905 58.317 48.182 1.00 42.68 ATOM 1620 C GLU A 210 19.905 58.311 47.381 1.00 40.30 ATOM 1620 C GLU A 210 19.905 58.311 47.381 1.00 40.30 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.89 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 ATOM 1622 CB GLU A 210 19.905 57.056 47.693 1.00 47.51 1.00 47.89 ATOM 1622 CB GLU A 210 19.905 57.056 47.6093 1.00 47.51 1.00 47.89 ATOM 1622 CB GLU A 210 20.884 59.553 47.613 1.00 42.01 ATOM 1622 CB GLU A 210 20.884 59.553 47.613 1.00 42.01 ATOM 1625 OGE GLU A 210 20.885 56.493 46.667 1.00 43.37 ATOM 1620 CD GER A 211 20.085 56.493		ATOM	1602	CA	GLY A	207	10.807	59.168	50.861	1.00 27.25
ATOM 1605 N ALA A 208 12.375 60.783 50.113 1.00 41.07 ATOM 1606 CA ALA A 208 13.370 61.354 49.233 1.00 42.72 ATOM 1607 C ALA A 208 14.660 60.550 49.356 1.00 49.10 ATOM 1608 O ALA A 208 15.651 60.997 49.957 1.00 51.30 ATOM 1609 CB ALA A 208 13.605 62.810 49.589 1.00 42.95 ATOM 1610 N LEU A 209 14.623 59.350 48.773 1.00 40.92 ATOM 1611 CA LEU A 209 15.739 58.440 48.825 1.00 39.55 ATOM 1612 C LEU A 209 16.756 58.575 47.743 1.00 47.96 ATOM 1613 O LEU A 209 16.756 58.575 47.743 1.00 47.96 ATOM 1614 CB LEU A 209 16.420 58.843 46.597 1.00 49.44 ATOM 1615 CG LEU A 209 14.420 56.803 50.129 1.00 40.46 ATOM 1616 CD1 LEU A 209 13.713 55.469 50.075 1.00 36.99 ATOM 1617 CD2 LEU A 209 15.283 56.921 51.387 1.00 43.31 ATOM 1618 N GLU A 210 17.999 58.317 48.182 1.00 42.68 50 ATOM 1620 C GLU A 210 19.205 58.311 47.381 1.00 47.89 ATOM 1620 C GLU A 210 19.965 57.056 47.693 1.00 47.51 ATOM 1621 O GLU A 210 19.965 57.056 47.693 1.00 47.89 ATOM 1622 CB GLU A 210 19.965 57.056 47.693 1.00 47.89 ATOM 1624 CD GLU A 210 19.965 57.056 47.693 1.00 47.89 ATOM 1627 N SER A 211 20.629 61.968 47.451 1.00 95.26 ATOM 1628 CA SER A 211 20.895 56.662 46.805 1.00 45.31 ATOM 1629 C SER A 211 23.143 55.535 46.3667 1.00 43.37 ATOM 1629 C SER A 211 23.649 56.423 46.366 1.00 44.33 ATOM 1630 O SER A 211 23.649 56.423 46.366 1.00 44.33 ATOM 1631 CB SER A 211 23.649 56.423 46.366 1.00 44.33 ATOM 1632 OG SER A 211 23.649 56.423 46.366 1.00 44.33 ATOM 1630 O SER A 211 23.649 56.423 46.366 1.00 44.33 ATOM 1630 O SER A 211 23.649 56.423 46.366 1.00 44.33 ATOM 1631 CB SER A 211 21.025 54.233 46.366 1.00 44.33 ATOM 1632 OG SER A 211 21.025 54.233 46.366 1.00 44.33 ATOM 1632 OG SER A 211 21.027 54.244 44.934 1.00 54.15		ATOM	1603	С	GLY A	207	11.802	59.632	49.838	1.00 38.81
ATOM 1605 N ALA A 208	235	ATOM	1604	0	GLY A	207	12.046	58.966	48.840	1.00 39.82
ATOM 1606 CA ALA A 208	line has	MOTA	1605	N	ALA A	208	12.375	60.783		
ATOM 1607 C ALA A 208 14.660 60.550 49.356 1.00 49.10 ATOM 1608 O ALA A 208 15.651 60.997 49.957 1.00 51.30 ATOM 1609 CB ALA A 208 13.605 62.810 49.589 1.00 42.95 ATOM 1610 N LEU A 209 14.623 59.350 48.773 1.00 40.92 ATOM 1611 CA LEU A 209 15.739 58.440 48.825 1.00 39.55 ATOM 1612 C LEU A 209 16.756 58.575 47.743 1.00 47.96 ATOM 1613 O LEU A 209 16.756 58.843 46.597 1.00 49.44 ATOM 1614 CB LEU A 209 16.420 56.803 50.129 1.00 40.46 ATOM 1615 CG LEU A 209 15.269 56.994 48.894 1.00 37.97 ATOM 1616 CD1 LEU A 209 15.269 56.994 48.894 1.00 37.97 ATOM 1617 CD2 LEU A 209 15.269 56.991 51.387 1.00 40.46 ATOM 1618 N GLU A 210 17.999 58.317 48.182 1.00 42.68 ATOM 1619 CA GLU A 210 17.999 58.311 47.381 1.00 40.30 ATOM 1620 C GLU A 210 19.205 58.311 47.381 1.00 47.51 ATOM 1621 O GLU A 210 19.965 57.056 47.693 1.00 47.51 ATOM 1623 CG GLU A 210 19.965 57.056 47.693 1.00 47.89 ATOM 1623 CG GLU A 210 19.965 57.056 47.693 1.00 47.89 ATOM 1623 CG GLU A 210 19.969 60.734 46.697 1.00 58.26 ATOM 1625 OEI GLU A 210 20.084 59.553 47.613 1.00 42.01 ATOM 1623 CG GLU A 210 20.084 59.553 47.613 1.00 42.01 ATOM 1623 CG GLU A 210 20.084 59.553 47.613 1.00 42.01 ATOM 1623 CG GLU A 210 20.084 59.553 47.613 1.00 42.01 ATOM 1627 N SER A 211 20.895 56.662 46.805 1.00 45.01 ATOM 1627 N SER A 211 20.895 56.662 46.805 1.00 45.01 ATOM 1629 C SER A 211 20.895 56.662 46.805 1.00 42.25 ATOM 1629 C SER A 211 23.143 55.535 46.667 1.00 43.37 ATOM 1620 C SER A 211 23.143 55.535 46.667 1.00 43.37 ATOM 1630 C SER A 211 23.649 56.493 46.086 1.00 44.33 ATOM 1631 CB SER A 211 23.649 56.493 46.086 1.00 44.33 ATOM 1631 CB SER A 211 23.649 56.493 46.086 1.00 44.33 ATOM 1631 CB SER A 211 23.649 56.493 46.086 1.00 44.33 ATOM 1631 CB SER A 211 23.649 56.493 46.086 1.00 44.33 ATOM 1631 CB SER A 211 23.649 56.493 46.346 1.00 44.33 ATOM 1631 CB SER A 211 23.244 54.244 44.934 1.00 54.15		ATOM	1606	CA	ALA A	208				
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ATOM 1620 C GLU A 210 19.965 57.056 47.693 1.00 47.51 ATOM 1621 O GLU A 210 19.708 56.432 48.721 1.00 47.89 ATOM 1622 CB GLU A 210 20.084 59.553 47.613 1.00 42.01 ATOM 1623 CG GLU A 210 19.699 60.734 46.697 1.00 58.26 ATOM 1624 CD GLU A 210 20.524 61.970 46.897 1.00100.00 ATOM 1625 OE1 GLU A 210 21.629 61.968 47.451 1.00 95.26 ATOM 1626 OE2 GLU A 210 19.935 63.047 46.486 1.00100.00 ATOM 1627 N SER A 211 20.895 56.662 46.805 1.00 45.01 ATOM 1628 CA SER A 211 21.661 55.442 47.013 1.00 42.25 ATOM 1630 O SER A 211 23.143 55.535 46.667 1.00 43.37 ATOM 1631 CB SER A 211 23.649 56.493 46.086 1.00 46.43 ATOM 1632 OG SER A 211 21.025 54.233 46.346 1.00 44.33 ATOM 1632 OG SER A 211 21.274 54.244 44.934 1.00 54.15	50	ATOM	1619	CA	GLU A	210	19.205	58.311	47.381	1.00 40.30
ATOM 1621 O GLU A 210 19.708 56.432 48.721 1.00 47.89 ATOM 1622 CB GLU A 210 20.084 59.553 47.613 1.00 42.01 ATOM 1623 CG GLU A 210 19.699 60.734 46.697 1.00 58.26 ATOM 1624 CD GLU A 210 20.524 61.970 46.897 1.00100.00 ATOM 1625 OE1 GLU A 210 21.629 61.968 47.451 1.00 95.26 ATOM 1626 OE2 GLU A 210 19.935 63.047 46.486 1.00100.00 ATOM 1627 N SER A 211 20.895 56.662 46.805 1.00 45.01 ATOM 1628 CA SER A 211 21.661 55.442 47.013 1.00 42.25 ATOM 1630 O SER A 211 23.143 55.535 46.667 1.00 43.37 ATOM 1631 CB SER A 211 23.649 56.493 46.086 1.00 46.43 ATOM 1632 OG SER A 211 21.025 54.233 46.346 1.00 44.33 ATOM 1632 OG SER A 211 21.274 54.244 44.934 1.00 54.15		ATOM	1620	С	GLU A	210	19.965	57.056	47.693	1.00 47.51
ATOM 1622 CB GLU A 210 20.084 59.553 47.613 1.00 42.01 ATOM 1623 CG GLU A 210 19.699 60.734 46.697 1.00 58.26 ATOM 1624 CD GLU A 210 20.524 61.970 46.897 1.00100.00 ATOM 1625 OE1 GLU A 210 21.629 61.968 47.451 1.00 95.26 ATOM 1626 OE2 GLU A 210 19.935 63.047 46.486 1.00100.00 ATOM 1627 N SER A 211 20.895 56.662 46.805 1.00 45.01 ATOM 1628 CA SER A 211 21.661 55.442 47.013 1.00 42.25 ATOM 1630 O SER A 211 23.143 55.535 46.667 1.00 43.37 ATOM 1631 CB SER A 211 23.649 56.493 46.086 1.00 46.43 ATOM 1632 OG SER A 211 21.025 54.233 46.346 1.00 44.33 ATOM 1632 OG SER A 211 21.274 54.244 44.934 1.00 54.15		ATOM	1621	0	GLU A	210			48.721	
ATOM 1623 CG GLU A 210 19.699 60.734 46.697 1.00 58.26 ATOM 1624 CD GLU A 210 20.524 61.970 46.897 1.00100.00 ATOM 1625 OE1 GLU A 210 21.629 61.968 47.451 1.00 95.26 ATOM 1626 OE2 GLU A 210 19.935 63.047 46.486 1.00100.00 ATOM 1627 N SER A 211 20.895 56.662 46.805 1.00 45.01 ATOM 1628 CA SER A 211 21.661 55.442 47.013 1.00 42.25 ATOM 1629 C SER A 211 23.143 55.535 46.667 1.00 43.37 ATOM 1630 O SER A 211 23.649 56.493 46.086 1.00 46.43 ATOM 1631 CB SER A 211 21.025 54.233 46.346 1.00 44.33 ATOM 1632 OG SER A 211 21.274 54.244 44.934 1.00 54.15				CB						
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ATOM 1632 OG SER A 211 21.274 54.244 44.934 1.00 54.15										
ATOM 1633 N ARG A 212 23.829 54.497 47.053 1.00 34.85									44.934	1.00 54.15
		MOTA	1633	N	ARG A	212	23.829	54.497	47.053	1.00 34.85

	ATOM	1634	CA	ARG A 212	25.229	54,328	46.791	1.00 35.41
	ATOM	1635	С	ARG A 212	25.430	52.838	46.567	1.00 45.39
	ATOM	1636	0	ARG A 212	24.840	52.027	47.276	1.00 48.85
	ATOM	1637	СВ	ARG A 212	26.101	54.846	47.915	1.00 37.25
5	ATOM	1638	CG	ARG A 212	27.151	55.827	47.402	1.00 68.10
•	ATOM	1639	CD	ARG A 212	26.532	56.962	46.587	1.00 76.55
	ATOM	1640	NE	ARG A 212	26.695	58.307	47.148	1.00 70.33
	ATOM	1641	CZ	ARG A 212	25.845	59.301	46.867	1.00 70.87
		1642		ARG A 212	24.806	59.105	46.059	1.00 70.87
10	ATOM							
10	ATOM	1643		ARG A 212	26.032	60.516	47.392	1.00 73.35
	ATOM	1644	N	GLN A 213	26.210	52.442	45.567	1.00 40.74
	ATOM	1645	CA	GLN A 213	26.408	51.021	45.331	1.00 39.90
	ATOM	1646	C	GLN A 213	27.646	50.537	46.050	1.00 46.34
1.5	ATOM	1647	0	GLN A 213	28.740	50.981	45.741	1.00 53.77
15	ATOM	1648	CB	GLN A 213	26.545	50.741	43.846	1.00 40.99
	MOTA	1649	CG	GLN A 213	26.976	49.296	43.532	1.00 55.79
	ATOM	1650	CD	GLN A 213	26.292	48.743	42.301	1.00 76.04
	MOTA	1651	OE1	GLN A 213	26.275	47.523	42.102	1.00 86.66
e ^{ra} Fig.	MOTA	1652	NE2	GLN A 213	25.700	49.618	41.489	1.00 55.45
-20	MOTA	1653	N	ILE A 214	27.495	49.649	47.013	1.00 33.12
4	ATOM	1654	CA	ILE A 214	28.663	49.206	47.743	1.00 32.55
	MOTA	1655	С	ILE A 214	28.911	47.765	47.536	1.00 39.29
Şafta	ATOM	1656	0	ILE A 214	29.726	47.162	48.230	1.00 42.41
# 2013	ATOM	1657	СВ	ILE A 214	28.546	49,428	49.250	1.00 35.72
25	MOTA	1658	CG1		27.395	48.573	49.791	1.00 36.13
ing feet	ATOM	1659	CG2		28.344	50.911	49.598	1.00 35.79
LT.	ATOM	1660		ILE A 214	27.067	48.841	51.260	1.00 33.79
is in	MOTA	1661	N	GLY A 215	28.199	47.197	46.598	1.00 40.03
#	ATOM	1662	CA	GLY A 215	28.638	45.855	46.234	
-30	ATOM	1663	C	GLY A 215	27.970	45.405		1.00 34.88
							44.950	1.00 41.09
	MOTA	1664	0	GLY A 215	27.083	46.048	44.425	1.00 44.25
	ATOM	1665	N	PRO A 216	28.448	44.262	44.410	1.00 39.62
	ATOM	1666	CA	PRO A 216	27.890	43.720	43.197	1.00 39.69
22 22	MOTA	1667	С	PRO A 216	26.369	43.661	43.253	1.00 41.56
35	ATOM	1668	0	PRO A 216	25.655	43.817	42.240	1.00 44.35
Barne .	MOTA	1669	CB	PRO A 216	28.448	42.311	42.996	1.00 39.91
	MOTA	1670	CG	PRO A 216	29.377	41.993	44.164	1.00 41.54
	MOTA	1671	CD	PRO A 216	29.514	43.411	44.897	1.00 37.70
40	ATOM	1672	N	ARG A 217	25.846	43.398	44.477	1.00 31.04
40	MOTA	1673	CA	ARG A 217	24.421	43.328	44.652	1.00 29.22
	ATOM	1674	С	ARG A 217	23.928	44.109	45.872	1.00 38.24
	ATOM	1675	0	ARG A 217	22.861	43.885	46.368	1.00 40.69
	MOTA	1676	CB	ARG A 217	24.012	41.844	44.790	1.00 22.75
	ATOM	1677	CG	ARG A 217	25.221	40.963	45.109	1.00 40.77
45	MOTA	1678	CD	ARG A 217	24.828	39.774	45.985	1.00 34.08
	MOTA	1679	NE	ARG A 217	26.020	39.183	46.581	1.00 45.20
	MOTA	1680	CZ	ARG A 217	25.955	37.894	46.911	1.00 65.13
	MOTA	1681	NH1	ARG A 217	24.832	37.220	46.716	1.00 42.40
	MOTA	1682	NH2	ARG A 217	26.997	37.300	47.472	1.00 48.08
50	ATOM	1683	N	THR A 218	24.784	45.022	46.404	1.00 31.00
	ATOM	1684	CA	THR A 218	24.309	45.886	47.487	1.00 31.00
	MOTA	1685	С	THR A 218	24.128	47.319	47.021	1.00 43.60
	ATOM	1686	0	THR A 218	25.065	47.930	46.512	1.00 48.42
	ATOM	1687	CB	THR A 218	25.315	45.845	48.640	1.00 36.95
55	MOTA	1688		THR A 218	25.430	44.517	49.139	1.00 45.66
	ATOM	1689		THR A 218	24.826	46.751	49.766	1.00 34.17
	ATOM	1690	N	LEU A 219	23.099	48.018	47.431	1.00 39.19
	MOTA	1691	CA	LEU A 219	23.055			
	ATOM	1692	C	LEU A 219	22.713	49.452	47.315	1.00 38.18
60	ATOM	1693	0	LEU A 219		50.000	48.695	1.00 42.32
50					22.108	49.289	49.498	1.00 43.67
	ATOM	1694	CB	LEU A 219	21.927	49.841	46.356	1.00 37.05
	ATOM	1695	CG CD1	LEU A 219	22.386	50.657	45.168	1.00 39.31
	ATOM	1696		LEU A 219	23.670	50.064	44.613	1.00 40.57
	MOTA	1697	CD2	LEU A 219	21.283	50.619	44.131	1.00 29.39

	ATOM	1698	N	VAL A	220	23.066	51.241	48.976	1.00 35.01
	ATOM	1699	CA	VAL A		22.741	51.830	50.253	1.00 36.98
		1700							
	ATOM		С	VAL A		21.736	52.923	50.043	1.00 44.08
_	ATOM	1701	0	VAL A		21.959	53.835	49.256	1.00 46.60
5	ATOM	1702	CB	VAL A		23.965	52.346	51.028	1.00 44.95
	ATOM	1703	CG1	VAL A	4 220	23.675	52.428	52.516	1.00 43.16
	MOTA	1704		VAL A		25.138	51.382	50.828	1.00 47.70
	ATOM	1705	N	TRP A					
						20.622	52.818	50.731	1.00 41.98
	MOTA	1706	CA	TRP A		19.605	53.828	50.602	1.00 41.64
10	MOTA	1707	С	TRP A	A 221	19.464	54.612	51.872	1.00 42.40
	ATOM	1708	0	TRP A	1 221	19.461	54.060	52.960	1.00 45.56
	ATOM	1709	СВ	TRP A	221	18.256	53.245	50.186	1.00 41.24
	ATOM	1710	CG	TRP A		18.353	52.459		
								48.918	1.00 42.59
1.5	ATOM	1711		TRP A		18.888	51.225	48.793	1.00 45.35
15	ATOM	1712		TRP A		17.949	52.873	47.590	1.00 41.62
	MOTA	1713	NE1	TRP A	A 221	18.826	50.832	47.478	1.00 44.74
	MOTA	1714	CE2	TRP A	A 221	18.243	51.821	46.720	1.00 45.31
	ATOM	1715		TRP A		17.345	54.009	47.061	1.00 41.17
4***		1716		TRP A					
	MOTA					17.958	51.902	45.346	1.00 42.60
20	ATOM	1717	CZ3	TRP A		17.054	54.083	45.710	1.00 39.08
43	ATOM	1718	CH2	TRP A	A 221	17.360	53.040	44.864	1.00 38.48
}-#\ 	ATOM	1719	N	SER A	A 222	19.271	55.896	51.688	1.00 37.01
2 m	ATOM	1720	CA		A 222	19.017	56.846	52.748	1.00 38.05
\$ 7 10 1 10	ATOM	1721	C		A 222				
25						18.853	58.251	52.205	1.00 45.28
23	MOTA	1722	0		A 222	19.005	58.503	51.008	1.00 44.02
LT -	ATOM	1723	CB	SER A	A 222	20.098	56.816	53.820	1.00 39.07
j€ ∖	MOTA	1724	OG	SER A	A 222	21.322	57.149	53.229	1.00 42.36
瘘	ATOM	1725	N	GLU A	A 223	18.586	59.190	53.088	1.00 40.91
	ATOM	1726	CA		A 223	18.465	60.527	52.584	1.00 41.97
30	ATOM	1727	C		A 223				
T. 30						19.843	61.042	52.234	1.00 50.17
n.	ATOM	1728	0		A 223	20.829	60.701	52.863	1.00 52.02
	ATOM	1729	CB	GLU 1	A 223	17.856	61.483	53.597	1.00 43.06
See in .	ATOM	1730	CG	GLU I	A 223	16.364	61.262	53.861	1.00 51.71
	ATOM	1731	CD	GLU Z	A 223	15.799	62.478	54.545	1.00 84.51
35	MOTA	1732	OE1		A 223	15.905	63.610	54.085	1.00 56.82
()	ATOM	1733	OE2		A 223	15.244	62.222		
								55.705	1.00 88.87
	ATOM	1734	N		A 224	19.892	61.875	51.229	1.00 47.39
	ATOM	1735	CA		A 224	21.139	62.456	50.792	1.00 48.51
	ATOM	1736	С	LYS A	A 224	22.163	62.683	51.930	1.00 50.90
40	ATOM	1737	0	LYS A	A 224	23.382	62.569	51.736	1.00 51.55
	ATOM	1738	CB		A 224	20.843	63.736	49.986	1.00 51.58
	MOTA	1739	CG		A 224	22.039	64.648	49.723	1.00 81.16
	ATOM	1740	CD		A 224				
						21.954	65.397	48.392	1.00 97.82
. 45	MOTA	1741	CE		A 224	21.646	66.891	48.530	1.00100.00
45	MOTA	1742	NZ	LYS A	A 224	22.056	67.700	47.362	1.00100.00
	MOTA	1743	N	GLU 1	A 225	21.683	63.011	53.123	1.00 45.77
	ATOM	1744	CA	GLU A	A 225	22.607	63.309	54.199	1.00 46.00
	ATOM	1745	С	GLU 2	A 225	23.227	62.150	54.902	1.00 47.99
	ATOM	1746	Ō		A 225	24.107	62.354		
50								55.732	1.00 47.21
	ATOM	1747	CB		A 225	22.057	64.296	55.210	1.00 47.71
	ATOM	1748	CG		A 225	20.530	64.296	55.182	1.00 63.24
	ATOM	1749	CD	GLU Z	A 225	19.931	65.219	54.150	1.00 75.13
	MOTA	1750	OE1	GLU I	A 225	20.187	66.420	54.046	1.00 54.64
	MOTA	1751		GLU A		19.039	64.578	53.420	1.00 49.64
55	MOTA	1752	N		A 226	22.798			
7.7							60.949	54.564	1.00 43.92
	ATOM	1753	CA		A 226	23.340	59.772	55.224	1.00 43.91
	ATOM	1754	С		A 226	24.036	58.756	54.322	1.00 45.86
	ATOM	1755	0	GLN A	A 226	24.756	57.871	54.806	1.00 45.70
	ATOM	1756	СВ		A 226	22.252	59.084	56.063	1.00 45.27
60	ATOM	1757	CG		A 226	21.965	59.790	57.400	1.00 31.17
-	ATOM	1758	CD		A 226				
						21.297	61.155	57.302	1.00 44.48
	MOTA	1759		GLN :		21.823	62.149	57.820	1.00 37.36
	MOTA	1760		GLN		20.115	61.202	56.696	1.00 30.28
	MOTA	1761	N	VAL .	A 227	23.814	58.871	53.021	1.00 41.20

	MOTA	1762	CA	VAL A	227	24.406	57.947	52.071	1.00 43.13
	MOTA	1763	С	VAL A	227	25.884	57.670	52.261	1.00 50.55
	MOTA	1764	0	VAL A	227	26.298	56.518	52.480	1.00 53.01
	MOTA	1765	CB	VAL A	227	24.155	58.293	50.604	1.00 49.39
5	MOTA	1766	CG1	VAL A	227	24.319	57.029	49.771	1.00 48.89
	ATOM	1767		VAL A		22.752	58.851	50.421	1.00 50.47
	ATOM	1768	N	GLU A		26.696	58.718	52.170	1.00 44.08
	ATOM	1769	CA	GLU A		28.123	58.542	52.310	1.00 41.71
	MOTA	1770	С	GLU A		28.514	57.871	53.583	1.00 44.20
10	MOTA	1771	0	GLU A		29.227	56.868	53.589	1.00 44.88
	MOTA	1772	CB	GLU A		28.935	59.824	52.102	1.00 43.08
	MOTA	1773	CG	GLU A		29.153	60.161	50.611	1.00 64.74
	MOTA	1774	CD	GLU A		29.114	58.965	49.701	1.00 84.29
1.5	ATOM	1775		GLU A		29.975	58.107	49.685	1.00 84.36
15	MOTA	1776	OE2			28.064	58.951	48.917	1.00 73.81
	ATOM	1777	N	LYS A		28.066	58.423	54.685	1.00 39.79
	ATOM	1778	CA	LYS A		28.449	57.796	55.922	1.00 39.04
.000 000.	ATOM	1779	C	LYS A		27.949	56.375	55.930	1.00 40.38
20	MOTA	1780	0	LYS A		28.639	55.433	56.346	1.00 43.63
4720	ATOM	1781	CB	LYS A		28.129	58.585	57.187	1.00 39.79
41	MOTA	1782	CG	LYS A		28.903	58.072	58.394	1.00 63.75
last.	MOTA	1783	CD	LYS A		28.498	58.763	59.685	1.00 77.46
14 m/	ATOM	1784	CE	LYS A		29.677	59.084	60.593	1.00 94.73
-25	ATOM	1785 1786	NZ	LYS A		30.344	60.353	60.256	1.00100.00
	ATOM ATOM	1787	N CA	SER A		26.741	56.220	55.428	1.00 28.48
	ATOM	1788	CA	SER A		26.174	54.891	55.377	1.00 25.93
1-4 .	ATOM	1789	Ö	SER A		27.089 27.469	53.988 52.855	54.587 54.955	1.00 30.26
*	ATOM	1790	CB	SER A		24.824	54.927	54.694	1.00 28.48
30	MOTA	1791	OG	SER A		23.822	55.293	55.605	
	MOTA	1792	N	ALA A		27.436	54.536	53.459	1.00 41.60 1.00 31.13
n.	ATOM	1793	CA	ALA A		28.288	53.820	52.593	1.00 31.13
	ATOM	1794	C	ALA A		29.597	53.383	53.270	1.00 47.68
44 th	ATOM	1795	ő	ALA A		30.003	52.238	53.103	1.00 47.00
35	ATOM	1796	СВ	ALA A		28.406	54.518	51.257	1.00 34.39
Bann.	ATOM	1797	N	TYR A		30.256	54.246	54.060	1.00 40.77
	ATOM	1798	CA	TYR A		31.500	53.830	54.730	1.00 38.40
	ATOM	1799	С	TYR A	232	31.265	52.721	55.753	1.00 39.70
	MOTA	1800	0	TYR A	232	32.041	51.772	55.862	1.00 36.46
40	MOTA	1801	CB	TYR A	232	32.311	54.981	55.414	1.00 38.27
	MOTA	1802	CG	TYR A		33.497	54.525	56.303	1.00 42.36
	ATOM	1803		TYR A		34.755	54.238	55.753	1.00 46.41
	ATOM	1804		TYR A		33.373	54.394	57.691	1.00 40.99
	MOTA	1805		TYR A		35.835	53.815	56.534	1.00 47.23
45	ATOM	1806	CE2	TYR A		34.441	53.979	58.496	1.00 40.10
	ATOM	1807	CZ	TYR A		35.680	53.695	57.916	1.00 48.59
	MOTA	1808	OH	TYR A		36.734	53.282	58.698	1.00 51.92
	ATOM	1809	N	GLU A		30.191	52.883	56.519	1.00 35.75
50	ATOM	1810	CA	GLU A		29.835	51.984	57.606	1.00 34.55
30	MOTA	1811	C	GLU A		29.633	50.498	57.252	1.00 38.39
	ATOM	1812	0	GLU A		30.152	49.576	57.892	1.00 38.55
	ATOM	1813	CB	GLU A		28.673	52.623	58.414	1.00 34.48
	ATOM	1814	CG	GLU A		28.666	52.262	59.912	1.00 24.95
55	ATOM	1815	CD	GLU A		29.463	53.183	60.787	1.00 37.55
	ATOM	1816				29.408	54.410	60.741	1.00 55.33
	MOTA MOTA	1817 1818	N N	GLU A PHE A		30.216	52.518	61.619	1.00 40.65
	MOTA	1819	N CA	PHE A		28.867	50.282	56.202	1.00 33.02
	MOTA	1820	CA	PHE A		28.493	48.974	55.719	1.00 29.90
60	ATOM	1821	0	PHE A		29.341 28.883	48.398	54.592	1.00 34.69
	ATOM	1822	CB	PHE A		27.020	47.521 49.081	53.823	1.00 34.21
	ATOM	1823	CG	PHE A		26.215	49.081	55.293 56.394	1.00 30.23
	ATOM	1824		PHE A		26.518	49.732	57.739	1.00 30.32 1.00 31.50
	ATOM	1825		PHE A		25.151	50.605	56.102	
		1020	J.J.L	rum tr	232	~~.171	50.005	50.102	1.00 28.66

	MOTA	1826	CE1	PHE A		25.780	50.103	58.772	1.00 30.43
	ATOM	1827	CE2	PHE A	234	24.407	51.203	57.121	1.00 29.60
	ATOM	1828	CZ	PHE A	234	24.725	50.959	58.458	1.00 27.47
	ATOM	1829	N	SER A		30.571	48.874	54.476	1.00 29.55
5	ATOM	1830	CA	SER A		31.428	48.366	53.412	1.00 28.64
	ATOM	1831	С	SER A		31.387	46.858	53.338	1.00 30.38
	MOTA	1832	ō	SER A		31.166	46.252	52.282	1.00 30.30
	ATOM	1833	CB	SER A					
						32.861	48.787	53.604	1.00 31.15
10	ATOM	1834	OG	SER A		33.028	49.368	54.873	1.00 39.32
10	ATOM	1835	N	GLU A		31.698	46.299	54.504	1.00 22.49
	ATOM	1836	CA	GLU A		31.815	44.873	54.737	1.00 23.79
	MOTA	1837	C	GLU A		30.627	43.992	54.380	1.00 32.37
	MOTA	1838	0	GLU A		30.697	42.772	54.545	1.00 29.91
	MOTA	1839	CB	GLU A	236	32.305	44.529	56.134	1.00 24.06
15	ATOM	1840	CG	GLU A	236	33.491	45.403	56.585	1.00 22.96
	ATOM	1841	CD	GLU A	236	33.600	45.492	58.090	1.00 66.18
	ATOM	1842	OE1	GLU A	236	32.633	45.482	58.849	1.00 37.01
	ATOM	1843	OE2	GLU A	236	34.848	45.518	58.494	1.00 78.68
F 13	ATOM	1844	N	THR A		29.560	44.593	53.891	1.00 34.11
20	ATOM	1845	CA	THR A		28.384	43.823	53.539	1.00 33.69
44.8	ATOM	1846	C	THR A		28.644	42.609	52.644	1.00 33.33
41	MOTA	1847	Ö	THR A		28.517		53.048	
jak,							41.451		1.00 31.09
III.	ATOM	1848	CB	THR A		27.218	44.710	53.057	1.00 37.99
25	ATOM	1849	OG1	THR A		26.899	45.675	54.048	1.00 33.49
間形とり	ATOM	1850	CG2	THR A		25.995	43.862	52.744	1.00 25.66
	ATOM	1851	И	GLU A		29.020	42.854	51.409	1.00 29.69
Har Ho.	ATOM	1852	CA	GLU A		29.267	41.734	50.520	1.00 27.05
	MOTA	1853	С	GLU A		30.071	40.638	51.146	1.00 33.17
	MOTA	1854	0	GLU A		29.660	39.497	51.055	1.00 38.50
30 m	MOTA	1855	CB	GLU A	238	29.851	42.080	49.161	1.00 27.50
in the second	MOTA	1856	CG	GLU A	238	30.116	40.813	48.320	1.00 18.83
n,	MOTA	1857	CD	GLU A	238	28.902	40.297	47.596	1.00 41.67
	ATOM	1858	OE1	GLU A	238	27.848	40.909	47.464	1.00 33.59
	ATOM	1-859	OE2	GLU A	238	29.085	39.089	47.138	1.00 46.30
[2] [4]35	ATOM	1860	N	SER A		31.203	40.973	51.772	1.00 24.44
this and	ATOM	1861	CA	SER A		32.045	39.957	52.387	1.00 24.60
	ATOM	1862	C	SER A		31.245	39.060	53.344	1.00 35.72
	ATOM	1863	Ö	SER A		31.379	37.830	53.360	1.00 35.72
	ATOM	1864	CB	SER A		33.231	40.601	53.074	1.00 33.23
40	ATOM	1865	OG	SER A		32.747	41.590		1.00 29.14
	ATOM	1866	N	MET A				53.961	
	ATOM	1867				30.382	39.703	54.154	1.00 33.13
			CA	MET A		29.529	38.993	55.091	1.00 28.55
	ATOM	1868	C	MET A		28.603	38.075	54.325	1.00 35.65
15	ATOM	1869	0	MET A		28.435	36.926	54.689	1.00 35.99
45	ATOM	1870	СВ	MET A		28.736	39.945	55.993	1.00 26.50
	ATOM	1871	CG	MET A		29.691	40.675	56.910	1.00 27.57
	ATOM	1872	SD	MET A		28.871	41.986	57.833	1.00 32.91
	MOTA	1873	CE	MET A		30.040	42.085	59.183	1.00 28.47
50	MOTA	1874	N	LEU A		28.019	38.603	53.243	1.00 32.77
50	ATOM	1875	CA	LEU A	241	27.120	37.859	52.381	1.00 29.87
	MOTA	1876	C	LEU A		27.848	36.615	51.878	1.00 36.76
	ATOM	1877	0	LEU A	241	27.302	35.509	51.858	1.00 36.97
	ATOM	1878	CB	LEU A	241	26.715	38.753	51.196	1.00 29.71
	ATOM	1879	CG	LEU A		25.283	39.289	51.237	1.00 37.68
55	ATOM	1880	CD1	LEU A		25.174	40.552	50.389	1.00 35.76
	ATOM	1881		LEU A		24.309	38.257	50.673	1.00 45.60
	ATOM	1882	N	LYS A		29.114	36.806	51.468	1.00 34.76
	ATOM	1883	CA	LYS A		29.908	35.702		
	ATOM	1884	C	LYS A				50.972	1.00 33.62
60	ATOM	1885	0	LYS A		30.072	34.690	52.039	1.00 32.18
00						29.887	33.512	51.795	1.00 32.56
	ATOM	1886	CB	LYS A		31.292	36.069	50.468	1.00 38.43
	ATOM	1887	CG	LYS A		31.406	36.263	48.961	1.00 49.23
	ATOM	1888	CD	LYS A		31.160	37.721	48.536	1.00 88.36
	MOTA	1889	CE	LYS A	242	32.371	38.456	47.943	1.00100.00

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	MOTA	1890	NZ	LYS A	242	32.033	39.411	46.862	1.00100.00
	ATOM	1891	N	ILE A	243	30.428	35.154	53.227	1.00 30.87
		1892	CA	ILE A		30.627	34.229	54.359	1.00 31.70
	ATOM								
	MOTA	1893	С	ILE A		29.381	33.458	54.764	1.00 36.50
5	ATOM	1894	0	ILE A	243	29.458	32.303	55.119	1.00 39.33
	ATOM	1895	CB	ILE A	243	31.227	34.886	55.579	1.00 32.36
	ATOM	1896	CG1			32.630	35.337	55.222	1.00 32.09
		1897	CG2	ILE A		31.243	33.891	56.718	
	MOTA								1.00 28.26
• •	ATOM	1898		ILE A		33.035	36.578	55.981	1.00 20.09
10	ATOM	1899	N	ALA A	244	28.237	34.120	54.708	1.00 32.10
•	MOTA	1900	CA	ALA A	244	26.968	33.519	55.066	1.00 32.95
	ATOM	1901	С	ALA A		26.600	32.392	54.127	1.00 36.35
		1902	Ö	ALA A		26.074	31.358	54.546	
	ATOM								1.00 36.88
	MOTA	1903	CB	ALA A		25.858	34.576	55.123	1.00 34.02
15	ATOM	1904	N	GLU A	245	26.890	32.617	52.846	1.00 31.20
	MOTA	1905	CA	GLU A	245	26.614	31.635	51.818	1.00 29.26
	MOTA	1906	С	GLU A		27.360	30.354	52.092	1.00 35.18
				GLU A					
	ATOM	1907	0			26.849	29.276	51.800	1.00 36.21
	MOTA	1908	CB	GLU A	245	26.908	32.177	50.421	1.00 30.22
20	MOTA	1909	CG	GLU A	245	25.701	32.938	49.842	1.00 39.79
41	ATOM	1910	CD	GLU A	245	26.026	33.564	48.529	1.00 51.91
ul .	MOTA	1911	OE1	GLU A	245	26.945	34.351	48.358	1.00 34.19
	ATOM	1912	OE2		-	25.246	33.142	47.585	1.00 47.48
lat.		1913	N						
in of	ATOM			ASP A		28.570	30.484	52.680	1.00 32.29
25	ATOM	1914	CA	ASP A		29.417	29.350	53.033	1.00 30.70
सम्बुक्तर संदुक्तर	MOTA	1915	С	ASP A	246	28.848	28.645	54.230	1.00 35.47
	ATOM	1916	0	ASP A	246	28.881	27.417	54.347	1.00 37.08
}=#\	ATOM	1917	CB	ASP A	246	30.873	29.717	53.355	1.00 33.17
	ATOM	1918	CG	ASP A		31.709	28.473	53.413	1.00 64.49
[‡] ₄30	ATOM	1919		ASP A		31.934	27.789	52.437	1.00 67.15
*1									
7.1	MOTA	1920		ASP A		32.118	28.167	54.622	1.00 79.01
	MOTA	1921	N	LEU A		28.323	29.434	55.134	1.00 33.59
18 min. 19 min.	ATOM	1922	CA	LEU A	247	27.731	28.868	56.334	1.00 36.70
	ATOM	1923	С	LEU A	247	26.355	28.208	56.083	1.00 35.92
£35	MOTA	1924	0	LEU A	247	26.060	27.110	56.551	1.00 30.77
þ.	ATOM	1925	СВ	LEU A		27.562	29.954	57.435	1.00 38.34
F***	ATOM	1926	CG	LEU A					
						28.732	30.100	58.394	1.00 44.30
	MOTA	1927	CD1			29.341	28.738	58.641	1.00 48.20
	MOTA	1928	CD2	LEU A		29.779	31.013	57.815	1.00 35.25
40	ATOM	1929	N	GLY A	248	25.471	28.887	55.353	1.00 34.97
	MOTA	1930	CA	GLY A	248	24.160	28.315	55.181	1.00 36.00
	ATOM	1931	С	GLY A	248	23.754	27.976	53.778	1.00 37.99
	ATOM	1932	0	GLY A		22.637	27.524	53.526	1.00 38.13
	MOTA	1933	N	GLY A				52.849	
AE						24.637	28.158		1.00 30.74
45	ATOM	1934	CA	GLY A		24.203	27.852	51.526	1.00 30.15
	ATOM	1935	С	GLY A		23.918	29.131	50.759	1.00 38.91
*	MOTA	1936	0	GLY A	249	24.126	30.240	51.238	1.00 41.32
	ATOM	1937	N	PRO A	250	23.453	28.946	49.547	1.00 38.93
	MOTA	1938	CA	PRO A		23.173	30.021	48.639	1.00 38.03
50	MOTA	1939	C	PRO A		22.203	31.078	49.096	1.00 42.17
50				PRO A					
	ATOM	1940	0			21.258	30.823	49.840	1.00 45.20
	ATOM	1941	CB	PRO A		22.663	29.357	47.352	1.00 39.18
	MOTA	1942	CG	PRO A	250	22.952	27.864	47.436	1.00 41.01
	ATOM	1943	CD	PRO A	250	23.396	27.610	48.865	1.00 38.57
55	MOTA	1944	N	TYR A	251	22.486	32.275	48.600	1.00 35.37
	MOTA	1945	CA	TYR A	251	21.692	33.461	48.817	1.00 34.87
	ATOM	1946	c	TYR A		20.740	33.479	47.649	1.00 39.55
	ATOM	1947	0	TYR A		21.125	33.794	46.535	1.00 42.57
	MOTA	1948	CB	TYR A		22.540	34.759	48.790	1.00 35.07
60	MOTA	1949	CG	TYR A	251	21.711	35.980	49.119	1.00 35.25
	MOTA	1950	CD1	TYR A	251	21.341	36.229	50.441	1.00 33.14
	MOTA	1951		TYR A		21.260	36.846	48.121	1.00 37.98
	ATOM	1952		TYR A		20.575	37.341	50.781	1.00 28.05
	ATOM	1953		TYR A					
	MOM	1323	CE2	TIN A	231	20.492	37.967	48.443	1.00 40.05

	ATOM	1954	CZ	TYR A 251	20.16					42.84
	ATOM	1955	ОН	TYR A 251	19.40					39.70
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	ATOM	1961	CG1	VAL A 252	18.37	78 30.	605 4	7.643	1.00	28.15
	ATOM	1962	CG2	VAL A 252	16.63	L4 32.	234 4	8.405	1.00	30.93
10	ATOM	1963	N	TRP A 253				7.504	1.00	32.44
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	ATOM	1965	С	TRP A 253	17.46	58 37.	341 4	6.119	1.00	43.56
	MOTA	1966	0	TRP A 253	16.69	90 38.	119 4	5.568	1.00	46.70
. <u> </u>	MOTA	1967	CB	TRP A 253	16.89	98 37.	302 4	8.606	1.00	29.65
15	ATOM	1968	CG	TRP A 253	16.30	5 4 36.	369 4	9.625	1.00	30.19
	ATOM	1969	CD1	TRP A 253	17.0			0.413	1.00	32.81
	ATOM	1970		TRP A 253		39 36.	110 4	9.913	1.00	29.63
	ATOM	1971	NE1	TRP A 253	16.2	51 34.	794 5	1.194	1.00	30.69
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20	MOTA	1973	CE3	TRP A 253	13.7	39 36.	637 4	9.450	1.00	30.18
14 m	MOTA	1974	CZ2	TRP A 253	13.7	46 34.	657 5	1.433	1.00	30.31
	MOTA	1975	CZ3	TRP A 253	12.6	00 36.	164 4	9.958	1.00	31.14
ju fix	ATOM	1976	CH2	TRP A 253	12.5	79 35.	176 5	0.946	1.00	31.37
\$ 4 44 - 4 4 5 4 44	ATOM	1977	N	GLY A 254	18.69			5.675	1.00	42.35
25	ATOM	1978	CA	GLY A 254	19.1	01 37.		4.509		41.34
Ų1	ATOM	1979	С	GLY A 254	19.8	75 39.		4.858		45.47
je to	ATOM	1980	0	GLY A 254				4.671		45.89
	ATOM	1981	N	GLN A 255				5.351		41.86
粮 .	ATOM	1982	CA	GLN A 255	19.7			5.675		38.67
30	ATOM	1983	С	GLN A 255				7.153		40.18
	ATOM	1984	0	GLN A 255				7.659		38.67
M.	ATOM	1985	СВ	GLN A 255				4.836		37.82
	ATOM	1986	CG	GLN A 255				5.169		50.17
es m.	ATOM	1987	CD	GLN A 255				4.283		62.88
35	MOTA	1988	OE1					3.463		55.76
	MOTA	1989	NE2					4.479		34.97
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40	ATOM	1993	0	TYR A 256	21.9	63 44.	321 4	9.225	1.00	24.22
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45	ATOM	1998	CE1	TYR A 256	20.4	36 41.	396 5	3.599	1.00	25.80
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	MOTA	2001	OH	TYR A 256	21.1	53 42.	433 5	5.631	1.00	37.35
	MOTA	2002	N	ASP A 257		34 44.	613 4	19.463	1.00	23.26
50	ATOM	2003	CA	ASP A 257			.027 4	19.621	1.00	23.47
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ATOM 2095 CD1 TYR A 267 12.915 45.765 66.856 1.00 27.0		MOTA	2083		TYR A 267	14.298	46.903	65.121	1.00 25.07
A TOM 2086 CD2 TYR A 267									1.00 24.45
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15 ATOM 2095 N GLY A 269 17.637 46.676 63.228 1.00 23.2 ATOM 2096 CA GLY A 269 17.637 46.520 61.853 1.00 21.6 ATOM 2098 O GLY A 269 15.681 44.948 62.820 1.00 27.8 ATOM 2099 N MET A 270 15.735 45.154 60.528 1.00 27.8 ATOM 2100 CA MET A 270 14.615 44.267 60.176 1.00 27.8 ATOM 2101 C MET A 270 14.615 44.267 60.176 1.00 27.8 ATOM 2102 O MET A 270 14.656 43.555 58.874 1.00 33.8 ATOM 2102 O MET A 270 15.221 44.247 57.867 1.00 33.8 ATOM 2103 CB MET A 270 15.221 44.247 57.867 1.00 34.8 ATOM 2104 CG MET A 270 15.221 44.247 57.867 1.00 34.8 ATOM 2105 SD MET A 270 12.195 43.937 59.602 1.00 26.6 ATOM 2106 CE MET A 270 11.875 42.742 60.929 1.00 37.3 ATOM 2107 C GLU A 271 14.955 42.263 58.904 1.00 32.8 ATOM 2108 CA GLU A 271 14.955 42.263 58.904 1.00 33.8 ATOM 2109 C GLU A 271 14.097 40.285 56.107 1.00 42.6 ATOM 2111 CB GLU A 271 14.097 40.285 56.107 1.00 42.6 ATOM 2112 CG GLU A 271 14.607 39.218 58.760 1.00 33.8 ATOM 2113 CD GLU A 271 14.697 40.285 56.107 1.00 42.6 ATOM 2113 CD GLU A 271 14.586 40.436 60.884 1.00 33.3 ATOM 2113 CD GLU A 271 14.586 40.436 60.844 10.00 33.3 ATOM 2110 CB GLU A 271 14.697 40.285 56.107 1.00 42.6 ATOM 2113 CD GLU A 271 14.586 40.436 60.844 40.00 33.3 ATOM 2115 OE2 GLU A 271 14.586 40.436 60.844 40.00 33.3 ATOM 2116 N ASN A 272 13.978 42.543 56.052 1.00 33.3 ATOM 2117 CA ASN A 272 13.978 42.545 56.052 1.00 33.3 ATOM 2118 C ASN A 272 13.978 42.545 56.052 1.00 33.3 ATOM 2120 CB ASN A 272 14.811 42.613 53.351 1.00 33.4 ATOM 2121 CG GLU A 271 14.586 40.436 60.844 41.00 33.3 ATOM 2120 CB ASN A 272 11.667 44.453 55.935 1.00 42.5 ATOM 2120 CG ASN A 272 13.978 42.545 56.052 1.00 33.3 ATOM 2121 CG SCU A 271 14.991 39.428 60.219 1.00 25.6 ATOM 2121 CG SCU A 271 14.991 39.428 60.919 1.00 25.6 ATOM 2122 CD ASN A 272 13.978 42.545 56.052 1.00 33.3 ATOM 2126 C PRO A 273 13.978 40.989 50.372 1.00 34.6 ATOM 2127 O PRO A 273 13.978 40.999 50.372 1.00 34.6 ATOM 2128 CB PRO A 273 13.991 40.993 53.078 1.00 29.6 ATOM 2129 CG PRO A 273 13.991 40.993 53.078 1.00 29.6 ATOM 2131 C CYS A 274 15.571 41.433 50.431 1.00 27.					GLY A 268			62.836	1.00 32.99
ATOM 2098 O GLY A 269 ATOM 2098 O GLY A 269 ATOM 2099 N MET A 270 ATOM 2099 N MET A 270 ATOM 2100 CA MET A 270 ATOM 2101 C MET A 270 ATOM 2102 O MET A 270 ATOM 2103 CB MET A 270 ATOM 2103 CB MET A 270 ATOM 2103 CB MET A 270 ATOM 2104 CG MET A 270 ATOM 2105 CB MET A 270 ATOM 2106 CE MET A 270 ATOM 2107 CB MET A 270 ATOM 2108 CB MET A 270 ATOM 2108 CB MET A 270 ATOM 2108 CB MET A 270 ATOM 2107 N GLU A 271 ATOM 2108 CB GLU A 271 ATOM 2110 C GLU A 271 ATOM 2111 CB GLU A 271 ATOM 2112 CG GLU A 271 ATOM 2114 CB GLU A 271 ATOM 2115 OBE GLU A 271 ATOM 2116 N ASN A 272 ATOM 2116 CB ASN A 272 ATOM 2116 CB ASN A 272 ATOM 2117 CA ASN A 272 ATOM 2118 C ASN A 272 ATOM 2119 O ASN A 272 ATOM 2116 CB ASN A 272 ATOM 2116 CB ASN A 272 ATOM 2117 CB ASN A 272 ATOM 2118 CC ASN A 272 ATOM 2119 CB ASN A 272 ATOM 2111 CC ASN A 272 ATOM 2112 CG BASN A 272 ATOM 2113 CD GLU A 271 ATOM 2114 CB ASN A 272 ATOM 2115 OBE 2 GLU A 271 ATOM 2116 N ASN A 272 ATOM 2117 CA ASN A 272 ATOM 2118 C ASN A 272 ATOM 2119 O ASN A 272 ATOM 2119 O ASN A 272 ATOM 2119 O ASN A 272 ATOM 2119 CB ASN A 272 ATOM 2119 CB ASN A 272 ATOM 2119 CB ASN A 272 ATOM 2110 CB ASN A 272 ATOM 2111 CB ASN A 272 ATOM 2112 CCB ASN A 272 ATOM 2119 O ASN A 272 ATOM 2119 O ASN A 272 ATOM 2110 CB ASN A 272 ATOM 2110 CB ASN A 272 ATOM 2111 CB ASN A 272 ATOM 2112 CCB ASN A 272 ATOM 2120 CB ASN A 272 ATOM 2121 CG ASN A 273 ATOM 2120 CB ASN A 272 ATOM 213 CD CB ASN A 272 ATOM 213 CD CB ASN A 272 ATOM 214 CB ASN A 273 ATOM 215 CB ASN A 272 ATOM 2120 CB ASN A 273 ATOM 2121 CG ASN A 273 ATOM 2121 CG ASN A 273 ATOM 2123 ND2 ASN A 272 ATOM 2124 N PRO A 273 ATOM 2125 CC PRO A 273 ATOM 2126 CB ASN A 272 ATOM 2127 O PRO A 273 ATOM 2130 CD PRO A 273 ATOM 2130 CD PRO A 273 ATOM 2130 CD PRO A 273 ATOM 2131 N CWS A 274 ATOM 2134 C CWS A 274 ATOM 2135 CB CWS A 274 ATOM 2136 CB CWS A 274 ATOM 2137 N LEU A		ATOM	2095	N	GLY A 269	17.637	46.676		1.00 23.19
ATOM 2098 N MET A 270 15.681 44.948 62.820 1.00 20.1 ATOM 2099 N MET A 270 15.735 45.154 60.528 1.00 27.6 ATOM 2100 CA MET A 270 14.615 44.267 60.176 1.00 25.6 ATOM 2101 C MET A 270 14.615 44.267 60.176 1.00 25.6 ATOM 2102 O MET A 270 14.615 44.267 60.176 1.00 25.6 ATOM 2102 O MET A 270 15.221 44.247 57.667 1.00 34.6 ATOM 2103 CB MET A 270 15.221 44.247 57.667 1.00 34.6 ATOM 2104 CG MET A 270 13.247 44.936 60.028 1.00 26.6 ATOM 2105 SD MET A 270 11.875 42.742 60.929 1.00 37.3 ATOM 2106 CE MET A 270 10.720 41.621 60.082 1.00 35.3 ATOM 2107 N GLU A 271 14.995 42.263 58.904 1.00 35.3 ATOM 2108 CA GLU A 271 15.393 41.459 57.753 1.00 33.3 ATOM 2110 O GLU A 271 14.087 40.285 56.107 1.00 42.6 ATOM 2111 CB GLU A 271 14.087 40.285 56.107 1.00 42.6 ATOM 2112 CG GLU A 271 14.087 40.285 56.107 1.00 42.6 ATOM 2113 CD GLU A 271 14.087 40.285 56.107 1.00 42.6 ATOM 2113 CD GLU A 271 14.991 39.428 60.219 1.00 35.4 ATOM 2113 CD GLU A 271 14.991 39.428 60.219 1.00 35.4 ATOM 2113 CD GLU A 271 14.991 39.428 60.219 1.00 35.4 ATOM 2113 CD GLU A 271 14.987 42.535 56.052 1.00 35.6 ATOM 2114 OEI GLU A 271 13.699 38.393 60.757 1.00 25.8 ATOM 2115 OE2 GLU A 271 13.699 38.393 60.757 1.00 25.8 ATOM 2116 N ASNA 272 13.057 42.544 54.928 1.00 33.3 ATOM 2117 CA ASNA 272 13.057 42.544 54.928 1.00 33.3 ATOM 2112 CG ASNA 272 13.057 42.544 54.928 1.00 33.3 ATOM 2120 CB ASNA 272 13.057 42.545 56.552 1.00 35.6 ATOM 2121 CG ASNA 272 11.908 45.554 56.457 1.00 42.8 ATOM 2122 ODL ASNA 272 11.908 45.554 56.457 1.00 30.4 ATOM 2122 ODL ASNA 272 11.908 45.554 56.457 1.00 30.4 ATOM 2123 ND2 ASNA 272 11.908 45.554 56.457 1.00 30.4 ATOM 2124 N PRO A 273 13.935 40.373 51.910 1.00 24.3 ATOM 2125 CA PRO A 273 13.935 40.373 51.910 1.00 24.3 ATOM 2126 C PRO A 273 13.457 42.089 50.372 1.00 31.4 ATOM 2127 O PRO A 273 13.457 42.089 50.372 1.00 31.4 ATOM 2128 CB PRO A 273 13.457 42.089 50.372 1.00 31.4 ATOM 2130 CD PRO A 273 13.457 42.089 50.372 1.00 31.4 ATOM 2131 N LEU A 275 15.658 43.972 50.947 1.00 26.4 ATOM 2131 O CUS A 274 15.659 40.998 50.099 1.00 22.4 ATOM 2131	15	ATOM	2096	CA	GLY A 269	17.393	46.320	61.853	1.00 21.62
ATOM 2099 N MET A 270 15.735 45.154 60.528 1.00 27.6 ATOM 2101 C MET A 270 14.615 44.267 60.176 1.00 25.6 ATOM 2102 O MET A 270 14.956 43.585 58.874 1.00 33.6 ATOM 2103 CB MET A 270 15.221 44.247 57.867 1.00 34.6 ATOM 2104 CG MET A 270 15.221 44.247 57.867 1.00 34.6 ATOM 2105 SD MET A 270 12.195 43.937 59.602 1.00 26.6 ATOM 2106 CE MET A 270 12.195 43.937 59.602 1.00 28.6 ATOM 2107 N GLU A 271 14.956 43.585 58.904 1.00 35.3 ATOM 2108 CA GLU A 271 15.393 41.459 57.753 1.00 32.2 ATOM 2109 C GLU A 271 15.393 41.459 57.753 1.00 32.2 ATOM 2110 O GLU A 271 14.407 40.285 56.107 1.00 40.6 ATOM 2111 CB GLU A 271 14.607 40.285 56.107 1.00 40.6 ATOM 2113 CD GLU A 271 14.607 40.285 56.107 1.00 33.4 ATOM 2113 CD GLU A 271 14.586 40.436 60.844 1.00 37.2 ATOM 2114 OEI GLU A 271 14.586 40.436 60.844 1.00 37.2 ATOM 2115 OEE GLU A 271 14.586 40.436 60.844 1.00 37.2 ATOM 2116 N ASN A 272 13.978 42.545 56.052 1.00 35.3 ATOM 2116 N ASN A 272 13.978 42.545 56.052 1.00 35.3 ATOM 2117 CA ASN A 272 13.978 42.545 56.052 1.00 35.3 ATOM 2118 C ASN A 272 13.978 42.545 55.935 1.00 33.3 ATOM 2119 O ASN A 272 13.978 42.545 55.935 1.00 33.4 ATOM 2121 CG ASN A 272 13.978 42.545 55.935 1.00 33.4 ATOM 2121 CG ASN A 272 13.978 42.545 55.935 1.00 33.4 ATOM 2121 CG ASN A 272 13.978 42.545 55.935 1.00 33.4 ATOM 2121 CG ASN A 272 13.978 42.545 55.935 1.00 33.4 ATOM 2121 CG ASN A 272 13.978 42.048 53.702 1.00 34.4 ATOM 2122 ODL ASN A 272 13.978 42.048 53.702 1.00 34.4 ATOM 2123 ND2 ASN A 272 13.978 42.048 53.702 1.00 34.4 ATOM 2124 N PRO A 273 13.281 40.983 53.078 1.00 29.4 ATOM 2123 ND2 ASN A 272 11.667 44.453 55.935 1.00 42.9 ATOM 2124 N PRO A 273 13.935 40.373 51.910 1.00 24.2 ATOM 2123 CG PRO A 273 13.935 40.373 51.910 1.00 24.2 ATOM 2124 N PRO A 273 13.935 40.373 51.910 1.00 24.2 ATOM 2123 CG PRO A 273 13.935 40.373 51.910 1.00 24.2 ATOM 2124 N PRO A 273 13.935 40.373 51.910 1.00 26.3 ATOM 2134 O CUS A 274 16.699 42.206 49.373 1.00 26.3 ATOM 2135 CB CVS A 274 16.699 45.375 51.595 1.00 47.3 ATOM 2134 O CUS A 275 15.658 43.972 50.555 1.00 32. ATOM 2		ATOM	2097	С	GLY A 269	16.187	45.402	61.777	1.00 27.53
ATOM 2100 CA MET A 270 14.615 44.267 60.176 1.00 25.2 ATOM 2101 C MET A 270 14.956 43.585 58.874 1.00 33.2 ATOM 2102 O MET A 270 15.221 44.247 57.867 1.00 34.6 ATOM 2103 CB MET A 270 13.247 44.936 60.028 1.00 26.2 ATOM 2104 CG MET A 270 13.247 44.936 60.028 1.00 26.2 ATOM 2105 SD MET A 270 13.247 44.936 60.028 1.00 26.2 ATOM 2106 CE MET A 270 11.875 42.742 60.929 1.00 37.2 ATOM 2107 N GLU A 271 14.995 42.263 58.904 1.00 35.3 ATOM 2108 CA GLU A 271 15.393 41.459 57.753 1.00 33.3 ATOM 2109 C GLU A 271 14.499 41.382 56.567 1.00 40.8 ATOM 2110 O GLU A 271 14.087 40.285 56.107 1.00 42.6 ATOM 2111 CB GLU A 271 14.607 39.218 58.760 1.00 35.3 ATOM 2112 CG GLU A 271 14.586 40.436 60.844 1.00 37.2 ATOM 2114 OEI GLU A 271 14.586 40.436 60.844 1.00 37.2 ATOM 2115 OE2 GLU A 271 13.699 38.393 60.757 1.00 25.8 ATOM 2116 N ASN A 272 13.978 42.545 56.052 1.00 35.3 ATOM 2117 CA ASN A 272 13.978 42.545 56.052 1.00 35.3 ATOM 2117 CA ASN A 272 13.978 42.545 56.052 1.00 35.3 ATOM 2120 CB ASN A 272 13.978 42.545 54.928 1.00 35.3 ATOM 2121 CG ASN A 272 13.978 42.545 56.052 1.00 35.3 ATOM 2120 CB ASN A 272 13.978 42.545 56.052 1.00 35.3 ATOM 2121 CG ASN A 272 13.978 42.545 56.052 1.00 35.3 ATOM 2121 CG ASN A 272 13.978 42.545 56.052 1.00 35.3 ATOM 2122 CB ASN A 272 13.978 42.048 53.702 1.00 34.4 ATOM 2122 CB ASN A 272 13.978 42.545 56.052 1.00 34.4 ATOM 2122 CB ASN A 272 11.4811 42.613 53.351 1.00 33.4 ATOM 2121 CG CB ASN A 272 11.4811 42.613 53.351 1.00 33.4 ATOM 2122 CB ASN A 272 11.998 45.555 56.052 1.00 34.4 ATOM 2123 ND2 ASN A 272 11.998 45.555 56.052 1.00 34.4 ATOM 2124 N PRO A 273 13.935 40.373 51.910 1.00 26.2 ATOM 2125 CR PRO A 273 13.935 40.373 51.910 1.00 26.2 ATOM 2126 C PRO A 273 13.935 40.373 51.910 1.00 28.2 ATOM 2133 C CYS A 274 16.699 42.206 49.373 1.00 28.2 ATOM 2134 C CYS A 274 16.699 42.206 49.373 1.00 28.2 ATOM 2135 CB CYS A 274 16.699 42.206 49.373 1.00 30.4 ATOM 2136 C CYS A 274 16.699 42.206 49.373 1.00 30.4 ATOM 2137 C PRO A 273 11.899 45.250 53.772 1.00 32.2 ATOM 2138 C LEU		ATOM		0					1.00 20.14
20 ATOM 2101 C MET A 270 114.956 43.585 58.874 1.00 33.5 ATOM 2102 O MET A 270 15.221 44.247 57.867 1.00 34.5 ATOM 2103 CB MET A 270 15.221 44.247 57.867 1.00 34.5 ATOM 2104 CG MET A 270 12.195 43.937 59.602 1.00 28.6 ATOM 2105 SD MET A 270 11.875 42.742 60.929 1.00 37.3 ATOM 2106 CE MET A 270 10.720 41.621 60.082 1.00 35.3 ATOM 2107 N GLU A 271 14.995 42.263 58.904 1.00 32.3 ATOM 2108 CA GLU A 271 14.995 42.263 58.904 1.00 32.3 ATOM 2109 C GLU A 271 14.419 41.382 56.567 1.00 40.6 ATOM 2110 O GLU A 271 14.419 41.382 56.567 1.00 40.6 ATOM 2111 CB GLU A 271 14.607 39.218 58.760 1.00 35.3 ATOM 2112 CG GLU A 271 14.607 39.218 58.760 1.00 35.3 ATOM 2113 CD GLU A 271 14.607 39.218 58.760 1.00 35.3 ATOM 2114 OE1 GLU A 271 14.586 40.436 60.844 1.00 37.2 ATOM 2115 OE2 GLU A 271 14.586 40.436 60.844 1.00 37.2 ATOM 2116 N ASN A 272 13.057 42.554 54.928 1.00 35.3 ATOM 2117 CA ASN A 272 13.057 42.554 54.928 1.00 35.3 ATOM 2118 C ASN A 272 13.057 42.554 54.928 1.00 35.3 ATOM 2119 O ASN A 272 13.057 42.544 54.928 1.00 33.3 ATOM 2120 CB ASN A 272 14.811 42.613 53.351 1.00 33.4 ATOM 2121 CB ASN A 272 11.908 45.554 56.677 1.00 42.5 ATOM 2120 CB ASN A 272 11.908 45.554 56.677 1.00 42.5 ATOM 2121 CB ASN A 272 11.908 45.554 56.677 1.00 42.5 ATOM 2122 OD1 ASN A 272 11.908 45.554 56.475 1.00 35.3 ATOM 2123 ND2 ASN A 272 11.908 45.554 56.475 1.00 33.4 ATOM 2124 N PRO A 273 13.935 40.373 51.910 1.00 29.4 ATOM 2122 CB PRO A 273 13.935 40.373 51.910 1.00 29.4 ATOM 2123 CB PRO A 273 13.935 40.373 51.910 1.00 28. ATOM 2124 CB PRO A 273 13.935 40.373 51.910 1.00 28. ATOM 2133 C CYS A 274 16.327 42.649 53.351 1.00 30.4 ATOM 2134 O CYS A 274 15.571 41.333 50.431 1.00 27. ATOM 2135 CB CYS A 274 16.327 42.609 50.372 1.00 31.4 ATOM 2134 O CYS A 274 15.571 41.333 50.431 1.00 28. ATOM 2135 CB CYS A 274 15.571 41.333 50.431 1.00 28. ATOM 2136 CB CYS A 274 15.565 43.972 50.947 1.00 26. ATOM 2137 O LEU A 275 15.658 43.972 50.947 1.00 26. ATOM 2138 CA LEU A 275 15.659 45.250 53.772 10.00 32. ATOM 2136 CB CYS A 274 15.629 45.505 53.005 1.00 32. ATOM 21	71								1.00 27.81
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## ATOM 2109 C GLU A 271 14.419 41.382 56.567 1.00 40.6 ## ATOM 2110 O GLU A 271 14.087 40.285 56.107 1.00 42.6 ## ATOM 2111 CB GLU A 271 15.802 40.054 58.230 1.00 35.6 ## ATOM 2112 CG GLU A 271 14.607 39.218 58.760 1.00 33.3 ## ATOM 2113 CD GLU A 271 14.586 40.436 60.844 1.00 37.2 ## ATOM 2114 OE1 GLU A 271 14.586 40.436 60.844 1.00 37.2 ## ATOM 2115 OE2 GLU A 271 13.699 38.393 60.757 1.00 25.6 ## ATOM 2116 N ASN A 272 13.978 42.535 56.052 1.00 35.2 ## ATOM 2117 CA ASN A 272 13.978 42.535 56.052 1.00 35.2 ## ATOM 2118 C ASN A 272 13.057 42.544 54.928 1.00 33.2 ## ATOM 2119 O ASN A 272 13.787 42.048 53.702 1.00 34.4 ## ATOM 2120 CB ASN A 272 11.667 44.453 55.935 1.00 42.5 ## ATOM 2121 CG ASN A 272 11.667 44.453 55.935 1.00 42.5 ## ATOM 2122 ODI ASN A 272 11.908 45.554 56.475 1.00 24.5 ## ATOM 2124 N PRO A 273 13.281 40.983 53.078 1.00 24.5 ## ATOM 2125 CA PRO A 273 13.935 40.373 51.910 1.00 28.5 ## ATOM 2127 O PRO A 273 13.935 40.373 51.910 1.00 28.5 ## ATOM 2128 CB PRO A 273 13.935 50.372 1.00 31.4 ## ATOM 2129 CG PRO A 273 13.935 50.372 1.00 31.4 ## ATOM 2129 CG PRO A 273 13.935 50.372 1.00 30.4 ## ATOM 2129 CG PRO A 273 13.935 50.372 1.00 30.4 ## ATOM 2121 CG PRO A 273 13.935 50.372 1.00 30.4 ## ATOM 2122 CD PRO A 273 13.935 50.372 1.00 30.4 ## ATOM 2123 CD PRO A 273 13.935 40.373 50.371 1.00 28.5 ## ATOM 2124 N PRO A 273 13.935 50.372 1.00 30.4 ## ATOM 2125 CA PRO A 273 13.935 50.372 1.00 30.4 ## ATOM 2128 CB PRO A 273 13.935 50.372 1.00 30.4 ## ATOM 2138 CD PRO A 273 13.935 50.372 1.00 30.4 ## ATOM 2138 CD PRO A 273 13.935 50.375 50.372 1.00 30.4 ## ATOM 2133 C CYS A 274 16.069 42.206 49.373 1.00 28.5 ## ATOM 2133 C CYS A 274 16.327 43.604 49.800 1.00 28.5 ## ATOM 2133 C CYS A 274 16.327 43.604 49.800 1.00 28.5 ## ATOM 2133 C CYS A 274 16.327 43.604 49.800 1.00 28.5 ## ATOM 2133 C CYS A 274 16.369 40.798 47.340 1.00 38.5 ## ATOM 2133 C CYS A 274 16.369 40.798 47.340 1.00 38.5 ## ATOM 2133 C CYS A 274 16.659 40.798 47.340 1.00 38.5 ## A	ga Šiv								1.00 32.20
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ATOM 2112 CG GLU A 271 14.607 39.218 58.760 1.00 33.5 ATOM 2113 CD GLU A 271 14.291 39.428 60.219 1.00 25.6 ATOM 2114 OE1 GLU A 271 14.586 40.436 60.844 1.00 37.2 ATOM 2115 OE2 GLU A 271 13.699 38.393 60.757 1.00 25.6 ATOM 2116 N ASN A 272 13.679 42.535 56.052 1.00 35.2 ATOM 2117 CA ASN A 272 13.057 42.544 54.928 1.00 33.2 ATOM 2118 C ASN A 272 13.057 42.544 54.928 1.00 33.2 ATOM 2119 O ASN A 272 14.811 42.613 53.351 1.00 33.4 ATOM 2120 CB ASN A 272 12.441 43.947 54.719 1.00 30.6 ATOM 2121 CG ASN A 272 11.667 44.453 55.935 1.00 42.5 ATOM 2122 OD1 ASN A 272 11.908 45.554 56.475 1.00 47.6 ATOM 2123 ND2 ASN A 272 11.908 45.554 56.6475 1.00 47.6 ATOM 2124 N PRO A 273 13.281 40.983 53.078 1.00 29.6 ATOM 2125 CA PRO A 273 13.281 40.983 53.078 1.00 29.6 ATOM 2126 C PRO A 273 13.281 40.983 53.078 1.00 29.6 ATOM 2127 O PRO A 273 13.457 42.089 50.372 1.00 31.4 ATOM 2128 CB PRO A 273 13.457 42.089 50.372 1.00 31.4 ATOM 2129 CG PRO A 273 13.457 42.089 50.372 1.00 31.4 ATOM 2129 CG PRO A 273 11.829 39.237 52.365 1.00 30.5 ATOM 2130 CD PRO A 273 11.829 39.237 52.365 1.00 30.5 ATOM 2131 N CYS A 274 15.571 41.333 50.431 1.00 27.6 ATOM 2133 CD PRO A 273 11.829 39.237 52.365 1.00 30.5 ATOM 2131 CPRO A 273 11.829 39.237 52.365 1.00 30.5 ATOM 2133 C CYS A 274 16.069 42.206 49.373 1.00 28.6 ATOM 2134 O CYS A 274 16.069 42.206 49.373 1.00 28.6 ATOM 2135 CB CYS A 274 16.069 42.206 49.373 1.00 28.5 ATOM 2136 CG CYS A 274 16.069 42.206 49.373 1.00 28.5 ATOM 2137 N LEU A 275 15.658 43.972 50.947 1.00 26.6 ATOM 2138 CA LEU A 275 15.658 43.972 50.947 1.00 26.6 ATOM 2138 CA LEU A 275 15.658 43.972 50.947 1.00 26.6 ATOM 2139 C LEU A 275 15.658 45.250 53.772 1.00 32.600 4700 2144 CD2 LEU A 275 14.857 45.250 53.772 1.00 22.600 4700 2144 CD2 LEU A 275 14.867 47.735 51.239 1.00 26.6 ATOM 2141 CB LEU A 275 14.867 46.253 51.005 1.00 32.600 4700 2144 CD2 LEU A 275 14.867 47.735 51.239 1.00 26.6 ATOM 2144 CD2 LEU A 275 14.867 47.735 51.239 1.00 26.6		ATOM	2110	0	GLU A 271	14.087		56.107	1.00 42.02
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ATOM 2134 O CYS A 274 17.114 44.345 49.248 1.00 28.3 ATOM 2135 CB CYS A 274 15.121 42.347 48.145 1.00 32.3 ATOM 2136 SG CYS A 274 14.659 40.798 47.340 1.00 38.3 ATOM 2137 N LEU A 275 15.658 43.972 50.947 1.00 26.3 ATOM 2138 CA LEU A 275 15.789 45.315 51.535 1.00 29.3 ATOM 2139 C LEU A 275 15.857 45.279 53.059 1.00 32.3 ATOM 2140 O LEU A 275 14.859 45.250 53.772 1.00 32.3 ATOM 2141 CB LEU A 275 14.657 46.253 51.005 1.00 28.3 ATOM 2142 CG LEU A 275 14.847 47.735 51.239 1.00 26.3 ATOM 2143 CD1 LEU A 275 16.191 48.183 50.698 1.00 21.3 ATOM 2144 CD2 LEU A 275 13.712 48.478 50.554 1.00 31.3		MOTA	2132	CA	CYS A 274				1.00 28.17
ATOM 2135 CB CYS A 274 15.121 42.347 48.145 1.00 32.0 ATOM 2136 SG CYS A 274 14.659 40.798 47.340 1.00 38.0 ATOM 2137 N LEU A 275 15.658 43.972 50.947 1.00 26.0 ATOM 2138 CA LEU A 275 15.789 45.315 51.535 1.00 29.0 ATOM 2139 C LEU A 275 15.857 45.279 53.059 1.00 32.0 ATOM 2140 O LEU A 275 14.859 45.250 53.772 1.00 32.0 ATOM 2141 CB LEU A 275 14.657 46.253 51.005 1.00 28.0 ATOM 2142 CG LEU A 275 14.847 47.735 51.239 1.00 26.0 ATOM 2143 CD1 LEU A 275 16.191 48.183 50.698 1.00 21.0 ATOM 2144 CD2 LEU A 275 13.712 48.478 50.554 1.00 31.				C					1.00 27.35
55 ATOM 2136 SG CYS A 274 14.659 40.798 47.340 1.00 38. ATOM 2137 N LEU A 275 15.658 43.972 50.947 1.00 26. ATOM 2138 CA LEU A 275 15.789 45.315 51.535 1.00 29. ATOM 2139 C LEU A 275 15.857 45.279 53.059 1.00 32. ATOM 2140 O LEU A 275 14.859 45.250 53.772 1.00 32. ATOM 2141 CB LEU A 275 14.657 46.253 51.005 1.00 28. ATOM 2142 CG LEU A 275 14.847 47.735 51.239 1.00 26. ATOM 2143 CD1 LEU A 275 16.191 48.183 50.698 1.00 21. ATOM 2144 CD2 LEU A 275 13.712 48.478 50.554 1.00 31.									1.00 28.53
ATOM 2137 N LEU A 275 15.658 43.972 50.947 1.00 26. ATOM 2138 CA LEU A 275 15.789 45.315 51.535 1.00 29. ATOM 2139 C LEU A 275 15.857 45.279 53.059 1.00 32. ATOM 2140 O LEU A 275 14.859 45.250 53.772 1.00 32. ATOM 2141 CB LEU A 275 14.657 46.253 51.005 1.00 28. ATOM 2142 CG LEU A 275 14.847 47.735 51.239 1.00 26. ATOM 2143 CD1 LEU A 275 16.191 48.183 50.698 1.00 21. ATOM 2144 CD2 LEU A 275 13.712 48.478 50.554 1.00 31.	55								1.00 32.00
ATOM 2138 CA LEU A 275 15.789 45.315 51.535 1.00 29.1 ATOM 2139 C LEU A 275 15.857 45.279 53.059 1.00 32.1 ATOM 2140 O LEU A 275 14.859 45.250 53.772 1.00 32.1 ATOM 2141 CB LEU A 275 14.657 46.253 51.005 1.00 28.1 ATOM 2142 CG LEU A 275 14.847 47.735 51.239 1.00 26.1 ATOM 2143 CD1 LEU A 275 16.191 48.183 50.698 1.00 21.1 ATOM 2144 CD2 LEU A 275 13.712 48.478 50.554 1.00 31.1	33								
ATOM 2139 C LEU A 275 15.857 45.279 53.059 1.00 32.1 ATOM 2140 O LEU A 275 14.859 45.250 53.772 1.00 32.1 ATOM 2141 CB LEU A 275 14.657 46.253 51.005 1.00 28.1 ATOM 2142 CG LEU A 275 14.847 47.735 51.239 1.00 26.1 ATOM 2143 CD1 LEU A 275 16.191 48.183 50.698 1.00 21.1 ATOM 2144 CD2 LEU A 275 13.712 48.478 50.554 1.00 31.									
ATOM 2140 O LEU A 275 14.859 45.250 53.772 1.00 32. ATOM 2141 CB LEU A 275 14.657 46.253 51.005 1.00 28. ATOM 2142 CG LEU A 275 14.847 47.735 51.239 1.00 26. ATOM 2143 CD1 LEU A 275 16.191 48.183 50.698 1.00 21. ATOM 2144 CD2 LEU A 275 13.712 48.478 50.554 1.00 31.									
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ATOM 2143 CD1 LEU A 275 16.191 48.183 50.698 1.00 21. ATOM 2144 CD2 LEU A 275 13.712 48.478 50.554 1.00 31.									1.00 26.78
ATOM 2144 CD2 LEU A 275 13.712 48.478 50.554 1.00 31.				CD1				50.698	1.00 21.90
ATOM 2145 N THR A 276 17.062 45.244 53.570 1.00 29.									1.00 31.48
		ATOM	2145	N	THR A 276	17.062	45.244	53.570	1.00 29.67

		ATOM	2146	CA	THR A	276	17.225	45.198	54.996	1.00 30.47
		ATOM	2147	С	THR A		17.120	46.624	55.597	1.00 34.60
		ATOM	2148	Ö	THR A		17.766	47.588	55.129	1.00 31.01
		ATOM	2149	CB	THR A		18.508	44.397	55.387	
	5			OG1						1.00 30.98
•	,	ATOM	2150		THR A		18.224	43.030	55.512	1.00 42.01
		ATOM	2151	CG2	THR A		19.124	44.835	56.694	1.00 29.43
		ATOM	2152	N	PHE A		16.280	46.759	56.622	1.00 27.69
		ATOM	2153	СA	PHE A		16.164	48.034	57.274	1.00 28.92
_	_	MOTA	2154	С	PHE A	277	17.184	48.065	58.403	1.00 36.07
10	0	ATOM	2155	0	PHE A	277	17.337	47.088	59.131	1.00 34.57
		MO'TA	2156	CB	PHE A	277	14.791	48.265	57.901	1.00 30.17
		MOTA	2157	CG	PHE A	277	13.774	48.458	56.848	1.00 30.72
		ATOM	2158	CD1	PHE A		14.011	47.966	55.568	1.00 30.73
		ATOM	2159		PHE A		12.573	49.114	57.105	1.00 30.61
1:	5	MOTA	2160		PHE A		13.072	48.135	54.552	1.00 29.30
1.		ATOM	2161		PHE A		11.619	49.276	56.101	
			2162	CZ	PHE A		11.862			1.00 32.26
		ATOM						48.772	54.824	1.00 27.48
E A		ATOM	2163	N	VAL A		17.864	49.186	58.562	1.00 32.97
	^	ATOM	2164	CA	VAL A		18.839	49.338	59.614	1.00 32.66
2	U	MOTA	2165	С	VAL A		18.696	50.698	60.248	1.00 37.01
Age and		MOTA	2166	0	VAL A		18.251	51.635	59.599	1.00 37.16
]=#\		ATOM	2167	CB	VAL A	278	20.246	49.088	59.109	1.00 36.51
### ##################################		MOTA	2168	CG1	VAL A	278	20.173	47.967	58.086	1.00 37.40
2		ATOM	2169	CG2	VAL A	278	20.791	50.356	58.444	1.00 34.87
2	5	ATOM	2170	N	THR A		19.066	50.778	61.515	1.00 32.36
# ₩		ATOM	2171	CA	THR A		18.948	51.994	62.264	1.00 31.03
p.L.		ATOM	2172	C	THR A		20.121	52.883	62.035	1.00 37.42
161		ATOM	2173	ŏ	THR A		21.243	52.397	61.920	1.00 37.42
j=4x		ATOM	2174	СВ	THR A		18.885	51.695	63.759	1.00 39.87
n. 3	n	ATOM	2175	OG1			19.110			
45 1914	Ų							52.895	64.472	1.00 34.21
T.J		MOTA	2176		THR A		19.989	50.706	64.083	1.00 23.69
122		ATOM	2177	N	PRO A		19.845	54.187	62.000	1.00 30.07
C.		ATOM	2178	CA	PRO A		20.903	55.132	61.802	1.00 27.00
	_	MOTA	2179	С	PRO A		21.823	55.110	63.005	1.00 30.60
1. 3.	5	ATOM	2180	0	PRO A	280	22.951	55.588	62.934	1.00 30.20
		MOTA	2181	CB	PRO A	280	20.249	56.497	61.601	1.00 26.23
		MOTA	2182	CG	PRO A	280	18.769	56.337	61.889	1.00 28.07
		ATOM	2183	$^{\rm CD}$	PRO A	280	18.499	54.848	61.984	1.00 26.11
		ATOM	2184	N	THR A	281	21.348	54.509	64.112	1.00 27.82
4	0	ATOM	2185	CA	THR A	281	22.199	54.426	65.302	1.00 27.48
		ATOM	2186	С	THR A	281	23.372	53.523	65.073	1.00 31.37
		ATOM	2187	0	THR A		24.226	53.385	65.944	1.00 31.93
		ATOM	2188	CB	THR A		21.499	54.016	66.601	1.00 21.45
		ATOM	2189	OG1			21.021	52.681	66.524	1.00 33.18
4	5	ATOM	2190		THR A		20.388	54.994	66.874	1.00 9.89
_	-	ATOM	2191	N	LEU A		23.378	52.881	63.913	1.00 25.29
		ATOM	2192	CA	LEU A		24.473	51.993	63.586	
		ATOM	2193	C	LEU A					1.00 24.04
		ATOM	2194	o			25.682	52.790	63.049	1.00 34.74
. 5	0				LEU A		26.787	52.279	62.884	1.00 34.84
ر	U	ATOM	2195	CB	LEU A		24.063	51.038	62.464	1.00 22.14
		ATOM	2196	CG	LEU A		23.104	49.916	62.819	1.00 26.88
		ATOM	2197		LEU A		23.312	48.809	61.791	1.00 27.77
		ATOM	2198		LEU A		23.322	49.404	64.249	1.00 21.75
	_	MOTA	2199	N	LEU A		25.465	54.063	62.744	1.00 32.05
)	5	ATOM	2200	CA	LEU A		26.501	54.903	62.159	1.00 31.43
		MOTA	2201	С	LEU A	283	27.659	55.324	63.055	1.00 41.94
		MOTA	2202	0	LEU A	283	27.907	56.525	63.196	1.00 49.19
		MOTA	2203	CB	LEU A		25.861	56.117	61.418	1.00 29.55
	100	ATOM	2204	CG	LEU A		24.720	55.661	60.488	1.00 32.94
6	0	ATOM	2205		LEU A		23.933	56.811	59.869	1.00 33.48
	-	MOTA	2206		LEU A		25.232	54.716	59.409	1.00 33.48
		ATOM	2207	N N	ALA A		28.387		63.638	
		MOTA	2208	CA	ALA A		29.488	54.370 54.728		1.00 33.18
		ATOM		C					64.532	1.00 30.20
		ATOM	2209	Ų,	ALA A	204	30.655	55.492	63.922	1.00 31.97

	ATOM	2210	0	ALA A	284	31.411	56.165	64.642	1 00 21 40
	ATOM	2211	СВ	ALA A		29.973	53.544	65.336	1.00 31.40
	ATOM	2212	N	GLY A		30.801	55.371	62.605	1.00 29.60 1.00 27.10
	ATOM	2213	CA	GLY A		31.882	56.018	61.867	1.00 27.10
5	ATOM	2214	С	GLY A		33.174	55.194	61.910	1.00 29.77
	ATOM	2215	0	GLY A		34.264	55.649	61.544	1.00 39.23
	ATOM	2216	N	ASP A		33.022	53.951	62.363	1.00 41.21
	ATOM	2217	CA	ASP A		34.144	53.057	62.473	1.00 34.57
	MOTA	2218	С	ASP A		33.805	51.625	62.130	1.00 32.57
10	MOTA	2219	0	ASP A		34.609	50.743	62.325	1.00 29.27
	ATOM	2220	CB	ASP A		34.812	53.163	63.860	1.00 34.65
	MOTA	2221	CG	ASP A	286	34.081	52.447	64.945	1.00 41.93
	ATOM	2222	OD1	ASP A	286	33.008	51.893	64.765	1.00 45.21
	MOTA	2223	OD2	ASP A	286	34.714	52.492	66.087	1.00 35.67
15	ATOM	2224	N	LYS A	287	32.590	51.395	61.641	1.00 29.46
	ATOM	2225	CA	LYS A		32.199	50.038	61.272	1.00 31.62
	ATOM	2226	С	LYS A		31.976	49.060	62.437	1.00 37.91
10 m	ATOM	2227	0	LYS A		31.761	47.879	62.240	1.00 37.91
41 00	ATOM	2228	CB	LYS A		33.215	49.447	60.304	1.00 32.17
20	ATOM	2229	CG	LYS A		33.510	50.358	59.119	1.00 51.60
H= Ac	ATOM	2230	CD	LYS A		33.960	49.601	57.877	1.00 50.74
E FRO RESTRIC	ATOM	2231	CE	LYS A		35.290	50.105	57.328	1.00 63.80
अबुद्धाः इसक	ATOM	2232	NZ	LYS A		35.167	50.866	56.069	1.00 71.91
150 O.S.	ATOM	2233	N	SER A		32.168	49.575	63.647	1.00 31.58
□ 25	ATOM	2234	CA	SER A		32.079	48.737	64.810	1.00 27.15
1-4×	ATOM	2235	C	SER A		30.742	48.137	65.142	1.00 36.08
#	ATOM	2236	0	SER A		30.676	47.318	66.057	1.00 37.87
1-1,	ATOM	2237	CB	SER A		32.618	49.463	66.005	1.00 16.31
30	ATOM	2238	OG	SER A		31.659	50.443	66.312	1.00 29.71
T.	ATOM	2239	N	LEU A		29.669	48.529	64.460	1.00 29.34
F 147	ATOM	2240	CA	LEU A		28.351	47.979	64.794	1.00 24.70
	ATOM	2241	C	LEU A		27.792	47.105	63.686	1.00 32.97
	ATOM ATOM	2242	O	LEU A		26.591	46.766	63.648	1.00 30.35
35	ATOM	2243 2244	CB CG	LEU A		27.385	49.090	65.191	1.00 21.45
55	ATOM	2244		LEU A		27.954	49.887	66.347	1.00 22.99
	ATOM	2246		LEU A		26.881	50.769	66.950	1.00 20.66
	ATOM	2247	N	SER A		28.381 28.723	48.881	67.394	1.00 29.65
	ATOM	2248	CA	SER A		28.453	46.753 45.941	62.801	1.00 31.21
40	ATOM	2249	C	SER A		27.861	44.582	61.645	1.00 29.89
	ATOM	2250	ō	SER A		27.299	43.872	62.006 61.153	1.00 30.57
	MOTA	2251	CB	SER A		29.704	45.800	60.783	1.00 29.73
	ATOM	2252	OG	SER A		30.470	44.725	61.266	1.00 29.27 1.00 38.77
	ATOM	2253	N	ASN A		27.980	44.207	63.282	1.00 26.55
45	ATOM	2254	CA	ASN A	291	27.449	42.909	63.706	1.00 25.78
	ATOM	2255		ASN A		26.006	42.773	63.355	1.00 30.89
	ATOM	2256		ASN A		25.576	41.702	62.975	1.00 30.09
	ATOM	2257	CB	ASN A	291	27.725	42.503	65.157	1.00 28.48
50	ATOM	2258	CG	ASN A	291	26.910	43.313	66.119	1.00 33.33
50	ATOM	2259	OD1	ASN A	291	27.065	44.529	66.198	1.00 34.48
	ATOM	2260		ASN A		26.001	42.653	66.818	1.00 28.96
	ATOM	2261		VAL A		25.277	43.885	63.476	1.00 30.68
	ATOM	2262		VAL A		23.865	43.924	63.142	1.00 30.27
55	ATOM	2263		VAL A		23.667	43.619	61.669	1.00 32.61
23	ATOM	2264		VAL A		22.644	43.082	61.255	1.00 33.31
	ATOM	2265		VAL A		23.288	45.289	63.505	1.00 35.13
	ATOM	2266		VAL A		21.877	45.486	62.946	1.00 33.48
	ATOM	2267		VAL A		23.328	45.478	65.014	1.00 35.02
60	ATOM	2268		ILE A		24.653	43.975	60.861	1.00 27.92
00	ATOM ATOM	2269		ILE A		24.527	43.685	59.461	1.00 28.71
	ATOM	2270 2271		ILE A		24.658	42.159	59.296	1.00 35.03
	ATOM	2272		ILE A		23.860	41.475	58.624	1.00 38.34
	ATOM	2273		ILE A		25.554 25.608	44.438	58.606	1.00 33.84
				A	255	23.000	45.952	58.898	1.00 34.55

	MOTA	2274	CG2	ILE A 2	293	25.305	44.186	57.121	1.00 36.50
	ATOM	2275		ILE A 2		24.265	46.680	58.808	1.00 30.49
	ATOM	2276		ALA A 2		25.668	41.584	59.934	1.00 23.76
			N						
_	ATOM	2277	CA	ALA A 2		25.836	40.138	59.809	1.00 19.95
5	MOTA	2278	C	ALA A 2	294	24.559	39.409	60.165	1.00 27.33
	MOTA	2279	0	ALA A 2		24.183	38.422	59.505	1.00 25.48
			CB	ALA A 2		26.984	39.644	60.688	1.00 19.24
	ATOM	2280							
	ATOM	2281	N	HIS A 2		23.917	39.934	61.244	1.00 27.63
	ATOM	2282	CA	HIS A 2	295	22.666	39.414	61.797	1.00 26.83
10	ATOM	2283	С	HIS A 2	295	21.611	39.383	60.734	1.00 28.61
10	ATOM	2284	ō	HIS A 2		21.169	38.301	60.348	1.00 25.72
	MOTA	2285	CB	HIS A 2		22.148	40.175	63.028	1.00 27.98
	MOTA	2286	CG	HIS A 2	295	20.937	39.534	63.657	1.00 31.62
	ATOM	2287	ND1	HIS A 2	295	21.047	38.675	64.763	1.00 32.66
15	ATOM	2288	CD2	HIS A 2	295	19.602	39.643	63.338	1.00 30.92
. 10				HIS A 2		19.802			
	MOTA	2289					38.298	65.088	1.00 30.14
	MOTA	2290	NE2	HIS A 2	295	18.916	38.860	64.254	1.00 30.24
in,	MOTA	2291	N	GLU A 2	296	21.257	40.590	60.251	1.00 27.23
top) ren	ATOM	2292	CA	GLU A 2	296	20.266	40.749	59.195	1.00 25.98
20		2293	C	GLU A		20.533	39.790		
20	ATOM							58.056	1.00 32.73
e #RV	ATOM	2294	0	GLU A	296	19.628	39.081	57.561	1.00 31.88
u Án	ATOM	2295	CB	GLU A :	296	20.046	42.203	58.728	1.00 24.55
in in	ATOM	2296	CG	GLU A 2	296	19.892	43.148	59.936	1,00 23.16
gan;	ATOM	2297	CD	GLU A		18.939	42.632	60.991	1.00 53.50
25									
23	MOTA	2298		GLU A		17.964	41.956	60.700	1.00 23.99
न केंद्र	ATOM	2299	OE2	GLU A	296	19.237	43.006	62.233	1.00 32.77
	ATOM	2300	N	ILE A	297	21.803	39.745	57.675	1.00 25.37
a	MOTA	2301	CA	ILE A	297	22.195	38.870	56.599	1.00 22.64
=# ₀	ATOM	2302	С	ILE A	297	21.812	37.445	56.859	1.00 27.47
30	ATOM	2303	ŏ	ILE A		21.175	36.799	56.048	1.00 26.25
	ATOM	2304	CB	ILE A		23.672	38.963	56.302	1.00 24.19
	MOTA	2305		ILE A		23.920	40.140	55.355	1.00 25.28
FR)	ATOM	_ 2306	CG2	ILE A	297	24.079	37.686	55.626	1.00 20.77
ंशक सहित्र सं	ATOM	2307	CD1	ILE A	297	25.325	40.705	55.435	1.00 16.26
⁻¹ 35	ATOM	2308	N	SER A	298	22.226	36.947	58.012	1.00 28.23
	MOTA	2309	CA	SER A		21.939	35.569	58.377	1.00 25.04
		2310	C C						
	ATOM			SER A		20.467	35.235	58.298	1.00 26.21
	ATOM	2311	0	SER A		20.118	34.097	58.000	1.00 26.30
	ATOM	2312	CB	SER A	298	22.520	35.209	59.714	1.00 27.82
40	ATOM	2313	OG	SER A	298	23.890	35.552	59.714	1.00 35.98
	ATOM	2314	N	HIS A	299	19.599	36.230	58.562	1.00 22.17
	MOTA	2315	CA	HIS A		18.205	36.092	58.719	
									1.00 22.77
	MOTA	2316	С	HIS A		17.614	35.710	57.387	1.00 29.10
	MOTA	2317	0	HIS A	299	16.553	35.162	57.290	1.00 31.50
45	ATOM	2318	CB	HIS A	299	17.662	37.432	59.200	1.00 24.67
	ATOM	2319	CG	HIS A	299	17.053	37.338	60.602	1.00 29.10
	ATOM	2320		HIS A		16.190	36.368	60.975	1.00 30.70
	MOTA	2321		HIS A		17.196	38.233	61.667	1.00 32.39
	MOTA	2322	CE1	HIS A	299	15.811	36.675	62.233	1.00 30.41
-50	MOTA	2323	NE2	HIS A	299	16.397	37.783	62.674	1.00 31.74
	ATOM	2324	N	SER A	300	18.356	36.048	56.315	1.00 23.31
	ATOM	2325	CA	SER A		17.942	35.581	55.010	1.00 24.24
	ATOM	2326	С	SER A		17.879	34.050	54.977	1.00 34.13
	ATOM	2327	0	SER A		17.075	33.463	54.305	1.00 33.28
- 55	MOTA	2328	CB	SER A	300	18.941	36.092	53.965	1.00 27.31
	MOTA	2329	OG	SER A	300	18.947	37.519	53.962	1.00 49.96
	ATOM	2330	N	TRP A		18.773	33.411	55.752	1.00 33.09
	MOTA	2331	CA	TRP A		18.702	31.969	55.829	1.00 31.84
C O	ATOM	2332	С	TRP A		17.740	31.511	56.895	1.00 32.15
60	MOTA	2333	0	TRP A		16.764	30.876	56.620	1.00 27.05
	ATOM	2334	CB	TRP A	301	20.095	31.429	56.082	1.00 30.16
	ATOM	2335	CG	TRP A	301	20.791	31.421	54.801	1.00 32.02
	ATOM	2336		TRP A		20.787	30.393	53.859	1.00 35.05
	ATOM	2337		TRP A		21.496	32.520	54.202	1.00 30.84
	111 011	2001		~ * * * * * * * * * * * * * * * * * * *	~ · ·	21.400	72.740	22.402	. 4.00 30.04

ATOM 2338 NEI TRP A 301 21.415 30.732 52.722 1.00 33.29 ATOM 2340 CE3 TRP A 301 21.861 32.12 52.921 1.00 33.29 ATOM 2341 CZ2 TRP A 301 22.573 32.970 52.108 1.00 32.65 ATOM 2342 CZ3 TRP A 301 22.573 32.970 52.108 1.00 32.65 ATOM 2344 CZ3 TRP A 301 22.503 34.652 53.812 1.00 36.108 ATOM 2344 N THR A 302 18.042 31.864 58.146 1.00 36.108 ATOM 2344 C THR A 302 18.042 31.864 58.146 1.00 31.75 ATOM 2345 C THR A 302 18.042 31.865 58.146 1.00 31.75 ATOM 2346 C THR A 302 16.279 32.680 39.695 1.00 33.55 ATOM 2346 C THR A 302 16.279 32.680 39.695 1.00 33.55 ATOM 2349 C THR A 302 17.053 31.920 63.366 1.00 36.55 ATOM 2349 C THR A 302 17.053 31.920 63.666 1.00 36.55 ATOM 2349 C THR A 302 17.053 31.920 63.666 1.00 36.55 ATOM 2349 C THR A 302 17.053 31.920 63.666 1.00 36.55 ATOM 2349 C THR A 302 17.053 31.920 63.666 1.00 36.55 ATOM 2352 C THR A 302 17.053 31.920 63.666 1.00 36.55 ATOM 2352 C THR A 302 17.053 31.920 63.666 1.00 36.69 ATOM 2353 C THR A 302 18.544 29.555 59.667 1.00 17.10 ATOM 2355 N ANN A 304 13.908 33.322 59.163 1.00 25.28 ATOM 2355 C ANN A 304 13.936 31.801 57.195 1.00 28.99 ATOM 2355 C ANN A 304 13.936 31.801 57.195 1.00 28.05 ATOM 2355 C ANN A 304 13.936 31.801 57.195 1.00 28.05 ATOM 2356 C ANN A 304 13.936 31.801 57.195 1.00 28.05 ATOM 2357 C ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2358 C ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2358 C ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2359 C B ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2357 C ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2358 C ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2358 C ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2358 C ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2359 C B ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2359 C C ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2359 C C ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2359 C C ANN A 304 14.091 35.176 55.047 1.00 28.05 ATOM 2368 C ANN A 304 14.091 35.199 35.055 1.00 27.24 ATOM 2368 C ANN A 306 13.917 39.97 35.051 1.00 28.05 ATOM 2378 C ANN A 306 13.917		MOTA	2338	NET	מ ססידי	301	21.415	30.732	52.722	1.00 33.29
ATOM 2340 CE3 TRP A 301 21.811 33.790 54.631 1.00 32.65 ATOM 2342 C23 TRP A 301 22.577 32.970 52.108 1.00 36.105 ATOM 2343 CH2 TRP A 301 22.573 34.652 53.812 1.00 36.103 ATOM 2344 N TRR A 302 21.888 34.239 52.544 1.00 36.103 ATOM 2345 CA TRR A 302 18.042 31.864 58.146 1.00 31.77 ATOM 2346 C TRR A 302 18.042 31.864 59.215 1.00 36.556 ATOM 2346 C TRR A 302 16.759 33.590 60.330 1.00 36.556 ATOM 2347 O TRR A 302 16.759 33.590 60.330 1.00 36.556 ATOM 2348 CB TRR A 302 17.963 30.920 60.366 1.00 31.04 ATOM 2349 CG TRR A 302 18.542 29.555 59.967 1.00 17.105 ATOM 2345 CG TRR A 302 18.542 29.555 59.967 1.00 17.105 ATOM 2350 CG2 TRR A 302 18.542 29.555 59.967 1.00 17.105 ATOM 2351 N GLY A 303 13.908 33.236 59.483 1.00 21.598 ATOM 2355 C GLY A 303 13.908 33.236 59.483 1.00 21.598 ATOM 2355 C GLY A 303 13.908 33.236 59.483 1.00 22.528 ATOM 2355 N A SNA 304 13.363 34.101 55.875 1.00 26.99 ATOM 2357 C A ANA 304 13.363 34.101 55.875 1.00 28.05 ATOM 2359 CB ASNA 304 12.118 32.715 54.415 1.00 24.87 ATOM 2359 CB ASNA 304 14.091 35.176 55.056 1.00 24.17 ATOM 2359 CB ASNA 304 14.091 35.176 55.056 1.00 24.17 ATOM 2359 CB ASNA 304 14.091 35.176 55.056 1.00 24.17 ATOM 2359 CB ASNA 304 14.091 35.176 55.056 1.00 24.17 ATOM 2359 CB ASNA 304 14.091 35.176 55.056 1.00 24.17 ATOM 2366 CB ASNA 304 14.091 35.176 55.056 1.00 24.17 ATOM 2366 CB ASNA 304 14.091 35.176 55.056 1.00 24.17 ATOM 2367 CG A ASNA 304 14.091 35.176 55.056 1.00 24.17 ATOM 2368 CB LEU A 305 13.287 39.595 59.595 1.00 24.17 ATOM 2368 CB LEU A 305 13.887 30.677 54.415 1.00 24.87 ATOM 2368 CB LEU A 305 13.887 30.577 54.415 1.00 24.87 ATOM 2368 CB LEU A 305 13.987 30.593 52.411 1.00 24.02 ATOM 2367 CG VAL A 306 13.396 30.293 52.411 1.00 31.29 ATOM 2368 CB LEU A 305 13.396 30.293 52.412 1.00 28.23 ATOM 2368 CB LEU A 305 13.396 30.293 52.412 1.00 28.23 ATOM 2375 CB VAL A 306 13.396 30.297 59.306 1.00 27.34 ATOM 2387 CG VAL A 306 13.396 30.297 59.300 1.00 28.23 ATOM 2388 CB VAL A 306 13.396 30.297 59.300 1.00 28.23 ATOM 2389 CB VAL A 308 9.902 2										
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ATOM 2349 OCI THR A 302	10									
ATOM 2351 N GC2 THR A 302										
ATOM 2351 N GLY A 303 15.053 32.418 59.250 1.00 25.28 ATOM 2352 CA GLY A 303 13.908 33.236 59.483 1.00 21.59 ATOM 2355 N ASN A 303 13.908 33.236 59.483 1.00 21.59 ATOM 2355 N ASN A 304 13.936 33.389 58.163 1.00 26.18 ATOM 2355 CA ASN A 304 13.936 33.389 58.163 1.00 26.18 ATOM 2355 CA ASN A 304 13.936 33.891 57.195 1.00 28.07 ATOM 2355 CA ASN A 304 13.936 33.891 57.195 1.00 28.07 ATOM 2359 CB ASN A 304 13.141 32.839 55.056 1.00 28.97 ATOM 2359 CB ASN A 304 14.131 32.839 55.056 1.00 28.97 ATOM 2359 CB ASN A 304 14.133 36.499 55.757 1.00 37.80 ATOM 2360 CG ASN A 304 14.133 36.499 55.757 1.00 37.80 ATOM 2361 ODI ASN A 304 14.133 36.499 55.757 1.00 23.55 ATOM 2361 ODI ASN A 304 14.133 36.499 55.757 1.00 27.84 ATOM 2363 N LEU A 305 14.110 31.919 55.055 1.00 27.24 ATOM 2363 CC LEU A 305 13.987 30.677 54.306 1.00 27.24 ATOM 2366 C LEU A 305 13.987 30.677 54.306 1.00 27.24 ATOM 2366 C LEU A 305 13.281 29.665 55.121 1.00 31.29 ATOM 2366 C LEU A 305 15.807 30.199 52.603 1.00 22.62 ATOM 2367 CB LEU A 305 15.807 30.199 52.603 1.00 22.62 ATOM 2367 CB LEU A 305 15.807 30.199 52.603 1.00 22.62 ATOM 2367 CB LEU A 305 15.807 30.199 52.603 1.00 22.62 ATOM 2367 CB LEU A 305 15.807 30.199 52.603 1.00 22.62 ATOM 2367 CB LEU A 305 15.807 30.199 52.603 1.00 22.62 ATOM 2370 CD2 LEU A 305 15.807 30.199 52.603 1.00 22.92 ATOM 2370 CD2 LEU A 305 15.807 30.199 52.603 1.00 22.92 ATOM 2370 CD2 LEU A 305 15.807 30.199 52.603 1.00 23.29 ATOM 2370 CD2 LEU A 305 15.807 30.199 52.603 1.00 23.09 ATOM 2370 CD2 LEU A 305 15.807 30.199 52.603 1.00 22.29 ATOM 2370 CD2 LEU A 305 15.807 30.199 52.603 1.00 23.09 ATOM 2370 CD2 LEU A 305 15.807 30.199 52.603 1.00 23.09 ATOM 2370 CD2 LEU A 305 15.807 30.199 52.603 1.00 23.09 ATOM 2370 CD2 LEU A 305 15.807 30.199 52.603 1.00 23.09 ATOM 2370 CD2 LEU A 306 15.409 30.299 52.412 1.00 28.99 ATOM 2370 CD2 LEU A 306 15.409 30.299 52.412 1.00 28.99 ATOM 2370 CD2 LEU A 306 15.409 30.299 57.807 58.400 1.00 23.09 ATOM 2370 CD2 LEU A 306 12.509 52.809 57.807 1.00 23.507 58.400 23.500 58.600 59.300 59.000 59.000 59.000										
15 ATOM 2353 C GLY A 303 13.908 33.236 59.483 1.00 26.99 ATOM 2355 N ASN A 304 13.908 33.206 57.994 1.00 26.18 ATOM 2355 N ASN A 304 13.936 33.040 57.994 1.00 26.18 ATOM 2355 C ASN A 304 13.936 33.041 57.195 1.00 28.05 ATOM 2355 C ASN A 304 13.363 34.101 55.875 1.00 28.17 ATOM 2356 O ASN A 304 12.118 32.715 54.415 1.00 24.97 ATOM 2356 C ASN A 304 12.118 32.715 54.415 1.00 24.97 ATOM 2356 C ASN A 304 14.091 35.176 55.056 1.00 22.55 ATOM 2360 C ASN A 304 14.091 35.176 55.047 1.00 23.55 ATOM 2361 OD1 ASN A 304 14.133 36.499 55.757 1.00 37.80 ATOM 2362 ND2 ASN A 304 14.133 36.613 56.892 1.00 20.66 ATOM 2363 N LEU A 305 13.987 30.677 54.306 1.00 24.17 ATOM 2363 N LEU A 305 13.987 30.677 54.306 1.00 27.24 ATOM 2366 O LEU A 305 13.288 29.665 55.121 1.00 21.29 ATOM 2366 O LEU A 305 15.301 30.1919 53.967 1.00 27.22 ATOM 2366 C LEU A 305 15.805 30.593 52.603 1.00 27.23 ATOM 2368 CC LEU A 305 15.805 30.593 52.603 1.00 27.23 ATOM 2370 CD2 LEU A 305 17.289 30.293 52.412 1.00 29.23 ATOM 2371 N VAL A 306 13.711 29.528 56.347 1.00 27.25 ATOM 2373 C VAL A 306 13.711 29.528 56.347 1.00 27.92 ATOM 2373 C VAL A 306 13.711 29.528 56.347 1.00 27.93 ATOM 2373 C VAL A 306 13.711 29.528 56.347 1.00 27.94 ATOM 2373 C VAL A 306 13.711 29.528 56.347 1.00 27.94 ATOM 2373 N THR A 307 10.499 30.358 59.320 1.00 38.36 ATOM 2375 CG2 VAL A 306 13.712 99.887 51.549 1.00 13.784 ATOM 2376 CG1 VAL A 306 13.713 29.528 56.347 1.00 29.99 ATOM 2373 N THR A 307 10.499 30.358 59.920 1.00 28.40 ATOM 2376 CG THR A 307 9.799 29.715 60.446 1.00 31.08 ATOM 2380 C THR A 307 9.799 29.715 60.446 1.00 31.08 ATOM 2380 C THR A 307 9.799 29.715 60.446 1.00 31.08 ATOM 2380 C THR A 307 9.799 29.716 60.426 1.00 29.99 ATOM 2380 C THR A 307 9.799 29.716 60.406 1.00 29.99 ATOM 2380 C C ANN A 308 9.802 30.347 61.608 1.00 29.29 ATOM 2380 C C ANN A 308 9.802 30.358 59.320 1.00 28.14 ATOM 2380 C C LYS A 309 5.550 28.433 62.294 1.00 28.17 ATOM 2380 C LYS A 309 5.551 62.6975 62.247 1.00 28.57 ATOM 2399 C C LYS A 309 5.551 62.6975 62.459 1.00 22.85 ATOM 2399 C C LYS A 309 3.543 2										1.00 25.28
ATOM 2354 C GLY A 303 13.202 33.382 58.163 1.00 26.99 ATOM 2355 N ASN A 304 13.936 33.891 57.195 1.00 28.05 ATOM 2356 CA ASN A 304 13.936 33.891 57.195 1.00 28.05 ATOM 2357 C ASN A 304 13.141 32.639 55.056 1.00 28.99 ATOM 2359 CB ASN A 304 12.118 32.715 54.415 1.00 24.87 ATOM 2359 CB ASN A 304 12.118 32.715 54.415 1.00 24.87 ATOM 2360 CG ASN A 304 14.091 35.176 55.077 1.00 23.55 ATOM 2361 DDI ASN A 304 14.133 36.499 55.757 1.00 37.80 ATOM 2362 ND2 ASN A 304 14.133 36.499 55.757 1.00 27.62 ATOM 2363 N LEU A 305 13.630 36.613 56.892 1.00 20.66 ATOM 2364 CA LEU A 305 13.987 30.677 54.306 1.00 27.24 ATOM 2365 C LEU A 305 13.987 30.677 54.306 1.00 27.24 ATOM 2366 C LEU A 305 13.218 29.665 55.121 1.00 31.29 ATOM 2366 C LEU A 305 13.218 29.665 55.121 1.00 27.62 ATOM 2366 C LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2366 C LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2368 CG LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2369 CDI LEU A 305 17.289 30.293 52.412 1.00 28.91 ATOM 2370 CD2 LEU A 305 17.289 30.293 52.412 1.00 28.91 ATOM 2370 CD2 LEU A 305 17.289 30.293 52.412 1.00 29.91 ATOM 2371 N VAL A 306 13.114 29.528 56.347 1.00 27.52 ATOM 2372 CA VAL A 306 13.114 29.528 56.347 1.00 27.94 ATOM 2373 C VAL A 306 13.114 29.528 56.347 1.00 27.95 ATOM 2375 CB VAL A 306 13.306 30.217 59.110 1.00 28.32 ATOM 2376 CGI VAL A 306 13.134 28.652 57.327 1.00 37.24 ATOM 2377 CG2 VAL A 306 13.134 28.652 57.327 1.00 37.24 ATOM 2378 C THR A 307 10.29 9.9571 58.440 1.00 28.12 ATOM 2380 C THR A 307 9.729 29.517 58.440 1.00 28.94 ATOM 2381 C THR A 307 9.729 29.712 60.446 1.00 38.36 ATOM 2388 C B THR A 307 9.729 29.712 60.446 1.00 32.93 ATOM 2380 C THR A 307 9.729 29.712 60.446 1.00 32.93 ATOM 2380 C C SAN A 308 9.802 30.347 61.608 1.00 23.03 ATOM 2380 C C SAN A 308 9.802 30.347 61.608 1.00 22.82 ATOM 2380 C C SAN A 308 9.802 30.347 61.00 29.29 ATOM 2380 C C SAN A 308 9.802 30.347 61.00 20.26.61 ATOM 2380 C C LYS A 309 3.430 62.230 1.00 22.96 ATOM 2391 DL ASN A 308 9.802 30.347 61.00 20.28.61 ATOM 2392 C C LYS A 309 3.430 62.433 62.230	15		2352	CA	GLY A	303	13.908	33.236	59.483	1.00 21.59
20 ATOM 2355 N ASN A 304 13.936 33.891 57.195 1.00 28.05 ATOM 2356 CA ASN A 304 13.363 34.101 55.875 1.00 28.17 ATOM 2357 C ASN A 304 13.141 32.639 55.056 1.00 28.99 ATOM 2359 CB ASN A 304 12.118 32.715 54.415 1.00 24.87 ATOM 2359 CB ASN A 304 12.118 32.715 54.415 1.00 24.87 ATOM 2360 CG ASN A 304 14.103 35.176 55.077 1.00 23.55 ATOM 2361 ODI ASN A 304 14.133 36.499 55.757 1.00 37.80 ATOM 2363 N LEU A 305 13.987 30.6613 56.892 1.00 20.66 ATOM 2363 N LEU A 305 13.987 30.677 54.306 1.00 27.24 ATOM 2366 C LEU A 305 13.987 30.677 54.306 1.00 27.34 ATOM 2366 C LEU A 305 13.218 29.665 55.121 1.00 31.29 ATOM 2368 CG LEU A 305 15.805 30.593 52.603 1.00 27.24 ATOM 2368 CG LEU A 305 15.805 30.593 52.603 30.223 ATOM 2368 CG LEU A 305 15.805 30.593 52.603 30.32.33 ATOM 2370 CD2 LEU A 305 17.289 30.293 52.401 1.00 28.91 ATOM 2370 CD2 LEU A 305 17.289 30.293 52.601 1.00 27.75 ATOM 2371 N VAL A 306 13.134 28.652 57.327 1.00 29.99 ATOM 2375 CB VAL A 306 13.134 28.652 57.327 1.00 29.99 ATOM 2376 CG1 VAL A 306 13.134 28.652 57.327 1.00 29.99 ATOM 2376 CG1 VAL A 306 13.134 28.652 57.327 1.00 29.99 ATOM 2377 CG2 VAL A 306 13.134 28.652 57.327 1.00 31.78 ATOM 2378 N THR A 307 10.499 30.358 59.320 1.00 31.78 ATOM 2378 N THR A 307 10.499 30.358 59.320 1.00 31.78 ATOM 2380 C THR A 307 9.729 29.712 60.446 1.00 37.56 ATOM 2380 C THR A 307 9.729 29.712 60.446 1.00 37.56 ATOM 2381 O THR A 307 9.729 29.712 60.446 1.00 37.56 ATOM 2385 N ASN A 308 9.042 29.862 62.724 1.00 27.02 45 ATOM 2386 C A SN A 308 9.042 29.862 62.724 1.00 27.02 50 ATOM 2387 C A SN A 308 9.042 29.862 62.724 1.00 27.02 51 ATOM 2380 C THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2381 O THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2388 O ASN A 308 9.042 29.865 62.474 1.00 23.03 ATOM 2388 O ASN A 308 9.042 29.865 62.724 1.00 27.02 52 ATOM 2398 C B ASN A 308 9.194 30.790 63.972 1.00 23.97 ATOM 2398 C C LYS A 309 3.430 29.756 62.474 1.00 23.03 ATOM 2399 C C LYS A 309 3.430 29.756 62.474 1.00 23.05 ATOM 2399 C D LYS A 309 3.543 22.075 61.924 1.00 38.25 ATOM 2399 CD LYS A		ATOM	2353	С	GLY A	303	13.202			1.00 26.99
ATOM 2356 CA		ATOM	2354	0	GLY A	303	12.040	33.040	57.994	1.00 26.18
20 ATOM 2358 C ASN A 304		ATOM	2355	N	ASN A	304	13.936	33.891	57.195	1.00 28.05
ATOM 2359 CB ASN A 304		MOTA	2356	CA	ASN A	304	13.363	34.101	55.875	1.00 28.17
ATOM 2359 CB ASN A 304	20	MOTA	2357	С	ASN A	304	13.141	32.839	55.056	1.00 28.99
ATOM 2360 CG ASN A 304 14.091 35.176 55.047 1.00 23.7.80 ATOM 2361 ODI ASN A 304 14.133 36.499 55.757 1.00 37.80 ATOM 2362 ND2 ASN A 304 14.752 37.488 55.093 1.00 20.66 250 ATOM 2362 ND2 ASN A 304 14.752 37.488 55.093 1.00 27.24 ATOM 2363 N LEU A 305 14.110 31.919 55.055 1.00 27.24 ATOM 2364 CA LEU A 305 13.987 30.677 54.306 1.00 27.34 ATOM 2366 C LEU A 305 13.987 30.677 54.306 1.00 27.34 ATOM 2366 C LEU A 305 12.235 29.051 54.678 1.00 27.24 ATOM 2366 C LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2367 CB LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2368 CG LEU A 305 15.805 30.593 52.412 1.00 28.91 ATOM 2370 CD2 LEU A 305 17.289 30.293 52.412 1.00 28.91 ATOM 2371 N VAL A 306 13.711 29.528 56.347 1.00 27.75 ATOM 2373 C VAL A 306 13.134 28.652 57.327 1.00 29.99 ATOM 2373 C VAL A 306 13.306 30.217 59.110 1.00 28.32 ATOM 2375 CB VAL A 306 13.306 30.217 59.110 1.00 28.32 ATOM 2376 CG1 VAL A 306 13.306 30.217 59.110 1.00 28.32 ATOM 2377 CG2 VAL A 306 13.409 27.593 57.827 1.00 37.24 ATOM 2378 N THR A 307 10.499 30.358 59.320 1.00 28.14 ATOM 2380 C THR A 307 10.499 30.358 59.320 1.00 28.14 ATOM 2381 O THR A 307 10.499 30.358 59.320 1.00 28.14 ATOM 2383 OGI THR A 307 9.299 28.706 60.277 1.00 37.56 ATOM 2383 OGI THR A 307 9.299 29.712 60.446 1.00 34.06 ATOM 2383 OGI THR A 307 9.299 29.712 60.446 1.00 29.40 ATOM 2388 C A SN A 308 9.02 29.8706 60.277 1.00 30.30 ATOM 2388 O ASN A 308 9.02 29.8706 60.277 1.00 30.30 ATOM 2388 O ASN A 308 9.02 29.8706 60.277 1.00 30.30 ATOM 2388 O ASN A 308 9.02 30.347 61.608 1.00 22.96 ATOM 2389 CB ASN A 308 9.02 29.868 62.244 1.00 27.82 ATOM 2389 CB ASN A 308 9.09 28.658 62.244 1.00 23.96 ATOM 2399 CB ASN A 308 9.09 28.658 62.2474 1.00 23.96 ATOM 2399 CD LYS A 309 3.445 2.6975 62.4479 1.00 28.87 ATOM 2398 CG LYS A 309 3.445 2.6975 62.4479 1.00 28.87 ATOM 2398 CG LYS A 309 3.445 2.6975 62.4479 1.00 28.87 ATOM 2398 CG LYS A 309 3.445 2.6075 61.924 1.00 28.87 ATOM 2399 CD LYS A 309 3.445 2.6075 61.924 1.00 28.87 ATOM 2399 CD LYS A 309 3.445 2.6075 61.924 1.00 28.87	uil)	MOTA	2358	0	ASN A	304	12.118	32.715	54.415	1.00 24.87
ATOM 2361 OD1 ASN A 304 11.333 36.613 56.892 1.00 20.666 at 70 20.666	i i	MOTA	2359	CB	ASN A	304		35.176	55.047	1.00 23.55
25 ATOM 2362 ND2 ASN A 304 14.752 37.488 55.093 1.00 24.17 ATOM 2363 N LEU A 305 14.110 31.919 55.055 1.00 27.24 ATOM 2365 C LEU A 305 13.987 30.677 54.306 1.00 27.34 ATOM 2366 C LEU A 305 13.987 30.677 54.306 1.00 27.34 ATOM 2366 C LEU A 305 13.987 30.677 54.306 1.00 27.34 ATOM 2366 C LEU A 305 15.301 30.119 53.967 1.00 27.62 ATOM 2367 CB LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2368 CG LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2369 CD1 LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2370 CD2 LEU A 305 17.289 30.293 52.412 1.00 28.91 ATOM 2371 N VAL A 306 13.711 29.528 56.347 1.00 27.75 ATOM 2373 C VAL A 306 13.711 29.528 56.347 1.00 27.75 ATOM 2373 C VAL A 306 13.342 28.652 57.327 1.00 29.99 ATOM 2375 C VAL A 306 13.306 30.217 59.110 1.00 28.32 ATOM 2375 C VAL A 306 13.306 30.217 59.110 1.00 28.32 ATOM 2375 C VAL A 306 13.306 30.217 59.110 1.00 28.32 ATOM 2375 C VAL A 306 15.479 28.180 57.969 1.00 38.36 ATOM 2379 CA THR A 307 10.499 30.358 59.320 1.00 29.40 ATOM 2379 CA THR A 307 9.729 29.517 58.440 1.00 29.40 ATOM 2380 C THR A 307 9.729 29.517 58.440 1.00 29.40 ATOM 2381 C THR A 307 9.729 29.517 58.440 1.00 29.40 ATOM 2383 C B THR A 307 9.729 29.517 58.460 1.00 23.03 ATOM 2383 C B THR A 307 9.729 29.517 58.460 1.00 23.03 ATOM 2383 C B THR A 307 9.729 29.517 58.460 1.00 23.03 ATOM 2383 C B THR A 307 9.729 29.517 58.460 1.00 23.03 ATOM 2383 C B THR A 307 9.729 29.517 58.460 1.00 23.03 ATOM 2383 C B ASN A 308 9.802 30.347 61.608 1.00 27.55 ATOM 2389 CB ASN A 308 9.802 30.347 61.608 1.00 23.57 ATOM 2389 CB ASN A 308 9.505 33.190 64.400 1.00 23.57 ATOM 2389 CB ASN A 308 9.505 33.190 64.400 1.00 23.57 ATOM 2389 CB ASN A 308 9.505 33.190 64.400 1.00 23.57 ATOM 2389 CB ASN A 308 9.505 33.190 64.400 1.00 23.57 ATOM 2389 CB ASN A 308 9.505 33.190 64.400 1.00 23.57 ATOM 2399 ND2 ASN A 308 9.505 33.190 64.400 1.00 23.57 ATOM 2399 CD LYS A 309 4.514 29.380 62.474 1.00 22.88 ATOM 2399 CD LYS A 309 4.514 29.380 62.464 1.00 23.57 ATOM 2399 CD LYS A 309 4.514 29.380 62.464 1.00 23.57 ATOM 2399 CD LYS A 309 3.453 25	a gæt	ATOM	2360				14.133	36.499		1.00 37.80
## ATOM 2364 CA LEU A 305 13.987 30.677 54.306 1.00 27.34 ## ATOM 2366 C LEU A 305 12.235 29.051 54.678 1.00 31.29 ## ATOM 2366 C LEU A 305 12.235 29.051 54.678 1.00 29.23 ATOM 2367 CB LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2369 CD1 LEU A 305 15.805 30.593 52.603 1.00 32.23 ATOM 2369 CD1 LEU A 305 17.289 30.293 52.412 1.00 28.91 ATOM 2370 CD2 LEU A 305 14.951 29.887 51.549 1.00 41.51 ATOM 2371 N VAL A 306 13.711 29.528 56.347 1.00 27.75 ATOM 2373 C VAL A 306 13.711 29.528 56.347 1.00 29.99 ATOM 2373 C VAL A 306 12.578 29.527 58.403 1.00 31.78 ATOM 2373 C VAL A 306 12.578 29.527 58.403 1.00 31.78 ATOM 2375 CB VAL A 306 13.304 30.217 59.110 1.00 28.32 ATOM 2375 CB VAL A 306 13.306 30.217 59.910 1.00 28.32 ATOM 2375 CG VAL A 306 15.479 28.180 57.969 1.00 37.24 ATOM 2376 CG1 VAL A 306 15.479 28.180 57.969 1.00 37.24 ATOM 2378 N THR A 307 11.259 29.517 58.440 1.00 29.40 ATOM 2378 N THR A 307 11.259 29.517 58.440 1.00 29.40 ATOM 2380 C THR A 307 10.499 30.358 59.320 1.00 28.14 ATOM 2380 C THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2381 O THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2381 O THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2381 O THR A 307 9.729 29.712 60.446 1.00 32.03 ATOM 2381 O THR A 307 9.029 28.706 60.277 1.00 36.72 ATOM 2380 CG THR A 307 9.029 28.706 60.277 1.00 36.72 ATOM 2380 CG THR A 307 9.029 28.706 60.277 1.00 28.14 ATOM 2380 CG THR A 307 9.029 28.706 60.277 1.00 28.56 ATOM 2383 CG THR A 307 9.029 28.706 60.277 1.00 28.56 ATOM 2386 CA ASN A 308 9.002 30.347 61.608 1.00 29.29 ATOM 2387 C ASN A 308 9.002 30.347 61.608 1.00 29.29 ATOM 2387 C ASN A 308 9.002 30.347 61.608 1.00 23.03 ATOM 2380 CB ASN A 308 9.002 30.347 61.608 1.00 23.03 ATOM 2380 CB ASN A 308 9.002 30.347 61.608 1.00 23.03 ATOM 2389 CB ASN A 308 9.002 30.347 61.608 1.00 23.03 ATOM 2389 CB ASN A 308 8.056 32.608 62.818 1.00 23.70 ATOM 2389 CB ASN A 308 8.056 32.608 62.818 1.00 23.70 ATOM 2395 C LYS A 309 4.514 29.380 62.964 1.00 22.88 ATOM 2399 CB LYS A 309 3.430 29.756 62.474 1.00 22.88 ATOM 2399 CB LYS A 309 3.430 29.75	##	ATOM					13.630	36.613	56.892	1.00 20.66
## ATOM 2364 CA LEU A 305 13.987 30.677 54.306 1.00 27.34 ## ATOM 2366 C LEU A 305 12.235 29.051 54.678 1.00 31.29 ## ATOM 2366 C LEU A 305 12.235 29.051 54.678 1.00 29.23 ATOM 2367 CB LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2369 CD1 LEU A 305 15.805 30.593 52.603 1.00 32.23 ATOM 2369 CD1 LEU A 305 17.289 30.293 52.412 1.00 28.91 ATOM 2370 CD2 LEU A 305 14.951 29.887 51.549 1.00 41.51 ATOM 2371 N VAL A 306 13.711 29.528 56.347 1.00 27.75 ATOM 2373 C VAL A 306 13.711 29.528 56.347 1.00 29.99 ATOM 2373 C VAL A 306 12.578 29.527 58.403 1.00 31.78 ATOM 2373 C VAL A 306 12.578 29.527 58.403 1.00 31.78 ATOM 2375 CB VAL A 306 13.304 30.217 59.110 1.00 28.32 ATOM 2375 CB VAL A 306 13.306 30.217 59.910 1.00 28.32 ATOM 2375 CG VAL A 306 15.479 28.180 57.969 1.00 37.24 ATOM 2376 CG1 VAL A 306 15.479 28.180 57.969 1.00 37.24 ATOM 2378 N THR A 307 11.259 29.517 58.440 1.00 29.40 ATOM 2378 N THR A 307 11.259 29.517 58.440 1.00 29.40 ATOM 2380 C THR A 307 10.499 30.358 59.320 1.00 28.14 ATOM 2380 C THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2381 O THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2381 O THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2381 O THR A 307 9.729 29.712 60.446 1.00 32.03 ATOM 2381 O THR A 307 9.029 28.706 60.277 1.00 36.72 ATOM 2380 CG THR A 307 9.029 28.706 60.277 1.00 36.72 ATOM 2380 CG THR A 307 9.029 28.706 60.277 1.00 28.14 ATOM 2380 CG THR A 307 9.029 28.706 60.277 1.00 28.56 ATOM 2383 CG THR A 307 9.029 28.706 60.277 1.00 28.56 ATOM 2386 CA ASN A 308 9.002 30.347 61.608 1.00 29.29 ATOM 2387 C ASN A 308 9.002 30.347 61.608 1.00 29.29 ATOM 2387 C ASN A 308 9.002 30.347 61.608 1.00 23.03 ATOM 2380 CB ASN A 308 9.002 30.347 61.608 1.00 23.03 ATOM 2380 CB ASN A 308 9.002 30.347 61.608 1.00 23.03 ATOM 2389 CB ASN A 308 9.002 30.347 61.608 1.00 23.03 ATOM 2389 CB ASN A 308 8.056 32.608 62.818 1.00 23.70 ATOM 2389 CB ASN A 308 8.056 32.608 62.818 1.00 23.70 ATOM 2395 C LYS A 309 4.514 29.380 62.964 1.00 22.88 ATOM 2399 CB LYS A 309 3.430 29.756 62.474 1.00 22.88 ATOM 2399 CB LYS A 309 3.430 29.75	25	ATOM	2362	ND2				37.488	55.093	1.00 24.17
## ATOM 2365 C LEU A 305 13.218 29.665 55.121 1.00 31.29 ATOM 2366 O LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2368 CG LEU A 305 15.371 30.119 53.967 1.00 27.62 ATOM 2369 CD1 LEU A 305 15.805 30.593 52.603 1.00 32.23 ATOM 2370 CD2 LEU A 305 17.289 30.293 52.412 1.00 28.91 ATOM 2370 CD2 LEU A 305 14.951 29.887 51.549 1.00 41.51 ATOM 2371 N VAL A 306 13.711 29.528 56.347 1.00 27.75 ATOM 2372 CA VAL A 306 13.711 29.528 56.347 1.00 27.75 ATOM 2373 C VAL A 306 13.306 30.217 59.110 1.00 28.92 ATOM 2374 O VAL A 306 13.306 30.217 59.110 1.00 28.32 ATOM 2375 CB VAL A 306 13.306 30.217 59.110 1.00 28.32 ATOM 2376 CG1 VAL A 306 15.479 28.180 57.969 1.00 38.36 ATOM 2377 CG2 VAL A 306 15.479 28.180 57.969 1.00 38.36 ATOM 2378 N THR A 307 11.259 29.517 58.440 1.00 29.40 ATOM 2378 N THR A 307 10.499 30.358 59.320 1.00 28.14 ATOM 2380 C THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2381 O THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2381 O THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2382 CB THR A 307 9.729 29.712 60.446 1.00 34.06 ATOM 2383 OG1 THR A 307 9.729 29.712 60.446 1.00 23.03 ATOM 2385 N ASN A 308 9.029 30.358 59.330 1.00 12.55 ATOM 2386 CA ASN A 308 9.029 30.356 62.274 1.00 28.56 ATOM 2387 C ASN A 308 9.029 30.357 61.600 12.55 ATOM 2388 OG ASN A 308 9.042 29.862 62.724 1.00 27.82 ATOM 2388 O ASN A 308 9.042 29.862 62.724 1.00 27.82 ATOM 2389 CB ASN A 308 9.042 29.862 62.724 1.00 27.82 ATOM 2389 CB ASN A 308 9.042 29.862 62.724 1.00 23.57 ATOM 2389 CB ASN A 308 9.042 29.862 62.724 1.00 23.57 ATOM 2399 CB ASN A 308 9.042 29.862 62.724 1.00 23.57 ATOM 2399 CB ASN A 308 9.555 33.190 64.400 1.00 23.70 ATOM 2395 C LYS A 309 4.514 29.380 62.964 1.00 23.80 ATOM 2395 C LYS A 309 4.514 29.380 62.964 1.00 23.80 ATOM 2395 C LYS A 309 4.514 29.380 62.964 1.00 22.86 ATOM 2399 CD LYS A 309 5.551 26.975 62.459 1.00 22.86 ATOM 2399 CD LYS A 309 5.551 26.975 62.459 1.00 22.86 ATOM 2399 CD LYS A 309 5.551 26.975 62.459 1.00 23.875 ATOM 2399 CD LYS A 309 3.4	M.	ATOM								
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ATOM 2393 N LYS A 309 6.890 28.658 62.640 1.00 24.10 ATOM 2394 CA LYS A 309 5.502 28.433 62.230 1.00 23.40 ATOM 2395 C LYS A 309 4.514 29.380 62.964 1.00 28.17 ATOM 2396 O LYS A 309 3.430 29.756 62.474 1.00 22.88 ATOM 2397 CB LYS A 309 5.151 26.975 62.459 1.00 24.26 ATOM 2398 CG LYS A 309 4.036 26.478 61.555 1.00 28.57 ATOM 2399 CD LYS A 309 3.543 25.075 61.924 1.00 38.25 ATOM 2400 CE LYS A 309 3.475 24.112 60.739 1.00 78.39		ATOM		OD1	ASN A	308	9.505	33.190	64.400	1.00 23.70
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ATUM Z4U1 NZ LYS A 309 4.389 22.953 60.849 1.00 98.22										
		MOTA	2401	NZ	LYS A	. 309	4.389	22.953	60.849	1.00 98.22

	ATOM	2402	N	THR A 31	0	4.917	29.744	64.179	1.00	23.46
	ATOM	2403	CA	THR A 31	0	4.179	30.616	65.037	1.00	22.98
	MOTA	2404	С	THR A 31	0	5.142	31.336	65.922	1.00	31.43
	MOTA	2405	0	THR A 31	0	6.223	30.836	66.230	1.00	31.51
5	ATOM	2406	CB	THR A 31		3.104	29.917	65.871	1.00	34.01
	MOTA	2407	OG1	THR A 31		3.684	29.148	66.945	1.00	27.97
	MOTA	2408	CG2	THR A 31		2.174	29.114	64.956		24.58
	ATOM	2409	N	TRP A 31		4.733	32.527	66.299		29.82
	MOTA	2410	CA	TRP A 31		5.559	33.371	67.120	1.00	30.49
10	MOTA	2411	С	TRP A 31		6.044	32.692	68.381	1.00	26.99
	ATOM	2412	0	TRP A 31		7.015	33.101	68.971		25.15
	ATOM	2413	CB	TRP A 31		4.933	34.768	67.320		30.34
	ATOM	2414	CG	TRP A 31		4.706	35.412	66.001		30.63
	ATOM	2415		TRP A 31		3.514	35.785	65.490		32.07
15	MOTA	2416		TRP A 31	_	5.705	35.723	65.008		31.31
	MOTA	2417		TRP A 31		3.703	36.335	64.250		29.97
	ATOM	2418		TRP A 31		5.033	36.317	63.931		32.88
e il	ATOM	2419		TRP A 31		7.099	35.586	64.943		31.44
tani Jihoo	MOTA	2420		TRP A 31		5.721	36.771	62.804		31.56
20	ATOM	2421		TRP A 31		7.779	36.059	63.848		30.39
4D	MOTA	2422		TRP A 31		7.089	36.639	62.789		30.58
<u> -4</u> ,	ATOM	2423	N	ASP A 31		5.366	31.632	68.770		27.36
Hands	ATOM	2424	CA	ASP A 31		5.757	30.868	69.950		27.38
HANGE	ATOM	2425	C	ASP A 31		7.149	30.213	69.757		31.25
25	ATOM	2426	0	ASP A 31		7.826	29.802	70.718		27.07
Jak.	ATOM	2427	CB	ASP A 31		4.697	29.750	70.217		25.96
	MOTA	2428	CG	ASP A 31		3.432	30.230	70.872		27.42
# L.	ATOM	2429		ASP A 31 ASP A 31		3.197	31.396	71.102 71.208		28.97
30	ATOM ATOM	2430 2431	N	HIS A 31		2.623 7.562	29.265			29.33
-30	ATOM	2431	CA	HIS A 31		8.820	30.089 29.454	68.487 68.164		25.04
r.	ATOM	2432	C	HIS A 31		9.864	30.452	67.737		23.48 25.38
	ATOM	2433	Ö	HIS A 31		10.929	30.432	67.214		29.97
	ATOM	2435	CB	HIS A 31		8.588	28.245	67.209		25.00
-35	ATOM	2436	CG	HIS A 31		7.641	27.230	67.837		29.77
4 55	ATOM	2437		HIS A 31		8.087	26.183	68.635		31.37
	ATOM	2438		HIS A 31		6.279	27.152	67.808		31.31
	ATOM	2439		HIS A 31		7.015	25.509	69.039		28.91
	ATOM	2440		HIS A 3		5.913	26.066	68.559		29.40
40	ATOM	2441	N	PHE A 31		9.521	31.682	68.005		17.43
	MOTA	2442	CA	PHE A 31		10.345	32.810	67.701		17.16
	ATOM	2443	С	PHE A 31		11.852	32.523	67.812		26.01
	ATOM	2444	0	PHE A 31		12.669	32.922	66.963		30.40
	ATOM	2445	CB	PHE A 31	4	9.908	34.056	68.517	1.00	18.63
45	ATOM	2446	CG	PHE A 33	L4	10.592	35.351	68.113	1.00	20.10
	ATOM	2447	CD1	PHE A 3	14	10.712	35.697	66.768	1.00	21.80
	MOTA	2448		PHE A 3		11.129	36.214	69.070	1.00	22.60
	ATOM	2449		PHE A 3		11.337	36.890	66.400		24.74
50	ATOM	2450		PHE A 3		11.750	37.416	68.716		27.24
50	ATOM	2451	CZ	PHE A 3		11.857	37.756	67.368		24.97
	MOTA	2452	N	TRP A 3		12.235	31.828	68.861		19.66
	ATOM	2453	CA	TRP A 3		13.639	31.541	69.068		17.87
-	MOTA	2454	C	TRP A 3		14.292	30.775	67.953		28.55
5.5	ATOM	2455	0	TRP A 3		15.518	30.769	67.830		29.23
55	ATOM	2456	CB	TRP A 3		13.860	30.842	70.362		16.03
	ATOM	2457	CG	TRP A 3		13.613	29.408	70.161		19.64
	ATOM	2458		TRP A 3		12.428	28.787	70.247		22.39
	MOTA	2459		TRP A 3		14.599	28.430	69.876		21.70
60	MOTA	2460		TRP A 3		12.597	27.457	70.033		24.22
60	ATOM	2461		TRP A 3		13.934	27.205	69.801		27.96
	ATOM	2462		TRP A 3		15.976	28.481	69.681		22.89
	ATOM	2463		TRP A 3		14.631	26.018	69.547		27.76
	ATOM	2464		TRP A 3		16.651	27.321	69.421		23.16
	ATOM	2465	Cn2	TRP A 3	1.3	15.991	26.108	69.341	1.00	23.94

	ATOM	2466	N	LEU A	316	13.488	30.114	67.144	1.00 26.33
	ATOM	2467	CA	LEU A		14.092	29.400	66.067	1.00 25.44
			Ĉ	LEU A					
	ATOM	2468				14.666	30.443	65.129	1.00 33.21
-	ATOM	2469	0	LEU A		15.737	30.252	64.530	1.00 37.80
. 5	ATOM	2470	CB	LEU A	316	13.050	28.567	65.311	1.00 24.82
	ATOM	2471	CG	LEU A	316	12.663	27.242	65.956	1.00 27.62
	MOTA	2472		LEU A		11.574	26.552	65.106	1.00 22.30
	ATOM	2473		LEU A		13.897	26.344	66.097	
									1.00 27.03
10	MOTA	2474	И	ASN A		13.931	31.555	64.997	1.00 20.55
10	MOTA	2475	CA	ASN A		14.354	32.624	64.115	1.00 19.34
	MOTA	2476	С	ASN A	317	15.603	33.333	64.531	1.00 30.38
	ATOM	2477	0	ASN A	317	16.553	33.425	63.766	1.00 32.04
	ATOM	2478	CB	ASN A		13.273	33.682	63.838	1.00 14.82
	ATOM	2479	CG	ASN A		12.330	33.177	62.793	1.00 31.14
15									
15	ATOM	2480		ASN A		12.151	31.966	62.657	1.00 38.42
	ATOM	2481	ND2	ASN A		11.724	34.074	62.049	1.00 17.34
	ATOM	2482	N	GLU A	318	15.562	33.870	65.750	1.00 26.15
	ATOM	2483	CA	GLU A	318	16.624	34.648	66.358	1.00 20.23
#FFIX	ATOM	2484	С	GLU A		17.860	33.884	66.816	1.00 23.53
20	ATOM	2485	Ö	GLU A		19.006			
रुक्ते स ्री							34.273	66.554	1.00 26.34
42	ATOM	2486	CB	GLU A		15.998	35.484	67.456	1.00 19.11
]=A.	ATOM	2487	CG	GLU A		14.999	36.480	66.800	1.00 24.06
P.	ATOM	2488	CD	GLU A	318	15.615	37.391	65.758	1.00 40.32
網報	ATOM	2489	OE1	GLU A	318	16.833	37.559	65.612	1.00 21.24
25	ATOM	2490	OE2	GLU A		14.703	38.025	65.062	1.00 24.23
# 199k	ATOM	2491	N	GLY A		17.621		67.494	
							32.782		1.00 17.17
-	MOTA	2492	CA	GLY A		18.681	31.955	68.016	1.00 15.31
*	MOTA	2493	С	GLY A	319	19.673	31.601	66.953	1.00 24.07
B a	MOTA	2494	0	GLY A	319	20.860	31.897	67.080	1.00 28.47
30	MOTA	2495	N	HIS A	320	19.165	30.956	65.907	1.00 20.24
1.J	MOTA	2496	CA	HIS A		19.977	30.556	64.790	1.00 20.13
T.J		2497	C	HIS A					
Tan all " of Janes.	MOTA					20.678	31.759	64.142	1.00 24.97
	MOTA	2498	0	HIS A		21.855	31.700	63.739	1.00 23.54
13 25	ATOM	2499	CB	HIS A	320	19.143	29.737	63.791	1.00 20.57
35	ATOM	2500	CG	HIS A	320	18.662	28.426	64.349	1.00 22.57
F 77 1	ATOM	2501	ND1	HIS A	320	17.471	28.332	65.058	1.00 22.98
	ATOM	2502		HIS A		19.217	27.176	64.286	1.00 19.52
	ATOM	2503		HIS A		17.336	27.046	65.385	1.00 19.18
		2504		HIS A					
40	ATOM					18.368	26.329	64.952	1.00 18.12
40	ATOM	2505	N	THR A		19.958	32.875	64.053	1.00 21.61
	MOTA	2506	CA	THR A	321	20.543	34.056	63.478	1.00 22.16
	ATOM	2507	С	THR A	321	21.697	34.552	64.342	1.00 27.47
	ATOM	2508	0	THR A	321	22.789	34.825	63.836	1.00 26.64
	ATOM	2509	CB	THR A		19.470	35.097	63.113	1.00 27.88
45	ATOM	2510							
				THR A		18.403	34.392	62.523	1.00 27.92
	ATOM	2511		THR A		19.999	36.088	62.087	1.00 18.05
	ATOM	2512	N	VAL A		21.496	34.634	65.659	1.00 21.90
	MOTA	2513	CA	VAL A	322	22.610	35.054	66.470	1.00 19.44
	MOTA	2514	С	VAL A	322	23.762	34.071	66.285	1.00 24.43
50	MOTA	2515	0	VAL A	322	24.926	34.414	66.188	1.00 21.48
	ATOM	2516	CB	VAL A		22.218	35.185	67.928	1.00 20.92
	ATOM	2517		VAL A		23.406	35.644		1.00 20.32
								68.772	
	MOTA	2518		VAL A		21.093	36.200	68.048	1.00 20.01
	ATOM	2519	N	TYR A		23.427	32.811	66.197	1.00 27.08
55	ATOM	2520	CA	TYR A		24.446	31.803	66.013	1.00 26.26
	ATOM	2521	С	TYR A	323	25.222	32.036	64.728	1.00 28.26
	MOTA	2522	0	TYR A		26.431	31.894	64.643	1.00 27.51
	ATOM	2523	СВ	TYR A		23.804			
							30.407	66.020	1.00 25.74
(0	ATOM	2524	CG	TYR A		24.867	29.341	65.987	1.00 26.66
60	ATOM	2525		TYR A		25.539	28.957	67.150	1.00 29.09
	ATOM	2526	CD2	TYR A	323	25.199	28.713	64.789	1.00 24.52
	ATOM	2527	CE1	TYR A	323	26.530	27.974	67.157	1.00 22.56
	ATOM	2528		TYR A		26.178	27.722	64.770	1.00 25.31
	ATOM	2529	CZ	TYR A		26.846	27.370	65.944	1.00 29.19
	-11-011					20.040	27.370	VV. VII	200 23.13

	ATOM	2530	OH	TYR A 323	27.823	26.434	65.895	1.00 27.51
		2531	N	LEU A 324		32.408	63.702	1.00 24.82
	ATOM							
	ATOM	2532	CA	LEU A 324	25.135	32.638	62.439	1.00 26.04
	MOTA	2533	С	LEU A 324		33.952	62.417	1.00 30.92
5	ATOM	2534	0	LEU A 324	26.903	34.045	61.851	1.00 33.76
	ATOM	2535	СВ	LEU A 324	24.176	32.537	61.235	1.00 26.21
	ATOM	2536	CG	LEU A 324	23.916	31.112	60.778	1.00 28.46
	ATOM	2537		LEU A 324	22.752	31.109	59.791	1.00 28.95
	ATOM	2538	CD2	LEU A 324	25.169	30.508	60.151	1.00 26.54
10	ATOM	2539	N	GLU A 325	25.234	34.976	63.033	1.00 27.04
10								
	MOTA	2540	CA	GLU A 325	25.870	36.303	63.064	1.00 22.88
	ATOM	2541	С	GLU A 325	27.282	36.210	63.624	1.00 28.76
	ATOM	2542	0	GLU A 325	28.250	36.722	63.026	1.00 26.24
	ATOM	2543	CB	GLU A 325	25.016	37.365	63.759	1.00 22.01
15								
15	ATOM	2544	CG	GLU A 325	25.827	38.411	64.524	1.00 41.55
	MOTA	2545	CD	GLU A 32!	25.035	39.040	65.646	1.00 72.11
	MOTA	2546	OET	GLU A 325	23.866	38.764	65.862	1.00 41.88
	ATOM	2547	OE2	GLU A 325	25.719	39.922	66.350	1.00 67.15
p# fig	ATOM	2548	N	ARG A 326	27.349	35.479	64.755	1.00 27.84
20	ATOM	2549	CA	ARG A 326	28.551	35.213	65.511	1.00 28.10
Asim.	ATOM	2550	C	ARG A 326	29.604	34.457	64.771	1.00 30.90
4.	ATOM	2551	0	ARG A 320	30.763	34.747	64.976	1.00 33.93
la.								
	MOTA	2552	CB	ARG A 32	28.334	34.761	66.947	1.00 31.52
##\ ##\	ATOM	2553	CG	ARG A 326	27.645	35.864	67.726	1.00 22.20
205								
25	ATOM	2554	CD	ARG A 32		35.572	69.203	1.00 28.71
9 1999	ATOM	2555	NE	ARG A 32	5 26.727	36.673	69.830	1.00 23.82
LT.								
}=£.	ATOM	2556	CZ	ARG A 32		36.556	70.780	1.00 26.09
E	MOTA	2557	NH1	ARG A 32	5 25.443	35.388	71.305	1.00 23.16
摩								
	MOTA	2558	NHZ	ARG A 32		37.655	71.222	1.00 24.77
F-30	ATOM	2559	N	HIS A 32	7 29.221	33.511	63.918	1.00 29.85
#T &								
र्व कुर्ग	ATOM	2560	CA.	HIS A 32		32.777	63.120	1.00 30.52
	ATOM	2561	С	HIS A 32	7 30.778	33.738	62.085	1.00 35.50
4 * * * * * * * * * * * * * * * * * * *	ATOM	2562	0	HIS A 32		33.777	61.822	1.00 36.74
122								
₹±#(*	MOTA	2563	CB	HIS A 32	7 29.591	31.555	62.407	1.00 31.59
-35	ATOM	2564	CG	HIS A 32	7 29.764	30.259	63.176	1.00 34.51
ر در ا								
Harane .	ATOM	2565	NDI	HIS A 32	7 30.963	29.913	63.788	1.00 36.17
	ATOM	2566	CD2	HIS A 32	7 28.875	29.263	63.432	1.00 35.58
	MOTA	2567 ·	CEI	HIS A 32	7 30.778	28.740	64.384	1.00 35.27
	ATOM	2568	NE2	HIS A 32	7 29.532	28.322	64.191	1.00 35.56
40								
40	ATOM	2569	N	ILE A 32		34.549	61.511	1.00 31.10
	MOTA	2570	CA	ILE A 32	30.328	35.517	60.528	1.00 31.66
	ATOM	2571	С	ILE A 32			61.086	1.00 40.12
	ATOM	2572	0	ILE A 32	8 32.451	36.615	60.465	1.00 40.81
	ATOM	2573	CB	ILE A 32		36.379	59.998	1.00 32.94
AE					-			
45	ATOM	2574	CG1	ILE A 32	8 28.220	35.570	59.114	1.00 29.53
	ATOM	2575	CG2	ILE A 32	8 29.694	37.591	59.201	1.00 30.91
	MOTA	2576	CDI	ILE A 32		36.463	58.535	1.00 32.98
	MOTA	2577	N	CYS A 32	9 31.179	36.948	62.266	1.00 37.88
= -	ATOM	2578	CA	CYS A 32			62.851	1.00 39.54
50	ATOM	2579	С	CYS A 32	9 33.475	37.092	63.157	1.00 40.19
			0					
	ATOM	2580		CYS A 32		37.642	62.971	1.00 38.44
	ATOM	2581	CB	CYS A 32	9 31.607	38.509	64.083	1.00 42.61
	MOTA	2582	SG	CYS A 32			63.619	1.00 48.14
	MOTA	2583	N	GLY A 33	0 33.332	35.852	63.632	1.00 34.74
55	ATOM	2584	CA	GLY A 33			63.980	1.00 35.20
	ATOM	2585	С	GLY A 33	0 35.359	34.854	62.778	1.00 43.66
	ATOM	2586	0	GLY A 33			62.891	1.00 46.79
	MOTA	2587	N	ARG A 33	1 34.709	34.725	61.622	1.00 34.99
	ATOM	2588	CA	ARG A 33	1 35.416		60.392	1.00 33.19
60								
UU	MOTA	2589	С	ARG A 33			60.017	1.00 40.63
	ATOM	2590	0	ARG A 33	1 37.238	35.914	59.586	1.00 44.40
				ARG A 33				
	ATOM	2591	CB				59.269	1.00 31.29
	ATOM	2592	CG	ARG A 33	1 33.987	32.685	59.450	1.00 47.66
	ATOM	2593	CD	ARG A 33			58.622	1.00 70.36
	AL OF	2000	UD.	1 min 12 33	. 54.012	31.122	50.044	1.00 /0.36

	3.0034	2504	3777	7DC 7 3	221	24 463	21 051	E7 221	1 00	00 05
	MOTA	2594	NE	ARG A 3		34.461	31.851	57.221		80.25
	ATOM	2595	CZ	ARG A 3		33.615	31.023	56.628		.00.00
	MOTA	2596		ARG A 3		33.055	29.999	57.279	1.00	79.12
	ATOM	2597	NH2	ARG A 3	331	33.334	31.216	55.341	1.00	89.33
5	ATOM	2598	N	LEU A 3	332	35.342	36.926	60.172	1.00	32.14
	ATOM	2599	CA	LEU A 3	332	35.885	38.198	59.820		30.02
	ATOM	2600	С	LEU A 3		37.013	38.612	60.761		40.33
	ATOM	2601	Ō	LEU A 3		38.084	38.972	60.286		40.10
	ATOM	2602	CB	LEU A 3		34.772	39.262			
10			CG	LEU A 3				59.822		28.20
10	ATOM	2603				34.451	39.896	58.469		28.82
	MOTA	2604	CD1			35.007	39.063	57.341		23.73
	MOTA	2605		LEU A 3		32.947	40.114	58.306		29.76
	MOTA	2606	N	PHE A 3		36.744	38.557	62.091	1.00	37.69
	ATOM	2607	CA	PHE A 3	333	37.657	38.997	63.143	1.00	34.12
15	ATOM	2608	С	PHE A 3	333	38.251	37.956	64.035	1.00	37.99
	ATOM	2609	0	PHE A 3	333	39.015	38.293	64.925		41.67
	ATOM	2610	CB	PHE A 3		36.970	40.058	64.024		35.62
	ATOM	2611	CG	PHE A 3		36.209	41.003	63.138		39.09
4234	MOTA	2612		PHE A 3		36.887	41.923	62.332		43.22
20	ATOM	2613		PHE A 3		34.818	40.941			
a a		2614	CE1	PHE A 3				63.045		42.78
u)	ATOM					36.205	42.781	61.464		44.14
ļ.	MOTA	2615		PHE A 3		34.123	41.806	62.194		46.56
4****	ATOM	2616	CZ	PHE A 3		34.814	42.716	61.389	1.00	43.20
25	ATOM	2617	N	GLY A 3		37.908	36.706	63.865	1.00	34.36
25	ATOM	2618	CA	GLY A 3	334	38.507	35.705	64.763	1.00	32.89
IJħ	ATOM	2619	С	GLY A 3	334	37.582	34.985	65.767	1.00	32.67
F#	ATOM	2620	0	GLY A 3	334	36.641	35.540	66.340		33.48
F-100	ATOM	2621	N	GLU A 3		37.908	33.726	66.003		23.52
豫	ATOM	2622	CA	GLU A 3		37.196	32.875	66.931		18.13
30	ATOM	2623	c	GLU A 3		37.278	33.384	68.346		29.15
	ATOM	2624	ō	GLU A		36.357	33.124	69.112		34.14
n.	ATOM	2625	CB	GLU A 3		37.782	31.488			
ii : ₩.			CG					66.929		17.35
	ATOM	2626		GLU A 3		37.041	30.591	67.929		32.97
2 35	ATOM	2627	CD	GLU A 3		35.642	30.305	67.473		46.14
35	ATOM	2628	OE1	GLU A 3		35.093	30.944	66.588		39.31
er :	ATOM	2629	OE2	GLU A 3		35.080	29.317	68.132	1.00	32.80
	ATOM	2630	N	LYS A 3		38.370	34.077	68.706	1.00	24.53
	MOTA	2631	CA	LYS A	336	38.468	34.609	70.061	1.00	25.38
	ATOM	2632	С	LYS A 3	336	37.445	35.726	70.169	1.00	35.32
40	ATOM	2633	0	LYS A	336	36.908	36.004	71.233	1.00	38.14
	MOTA	2634	CB	LYS A 3	336	39.820	35.199	70.421		25.45
	MOTA	2635	CG	LYS A 3	336	40.871	34.188	70.825		25.43
	ATOM	2636	CD	LYS A		42.207	34.846	71.189		47.10
	ATOM	2637	CE	LYS A 3		43.325	34.600	70.172		68.74
45	ATOM	2638	NZ	LYS A		44.566	34.072	70.767		77.62
	ATOM	2639	N	PHE A		37.174	36.364	69.029		31.52
	ATOM	2640	CA	PHE A		36.186	37.442	68.967		
	ATOM	2641	C	PHE A		34.783	36.869			29.34
	MOTA	2642		PHE A				69.083		31.73
50		2643	0			33.908	37.424	69.742		35.53
50	ATOM		CB	PHE A		36.304	38.336	67.709		30.04
	ATOM	2644	CG	PHE A		35.435	39.589	67.747		35.16
	ATOM	2645		PHE A		35.468	40.459	68.843		43.88
	ATOM	2646		PHE A		34.550	39.893	66.709		40.16
	MOTA	2647		PHE A		34.688	41.617	68.913	1.00	46.53
55	ATOM	2648	CE2	PHE A	337	33.753	41.040	66.760	1.00	45.62
	ATOM	2649	CZ	PHE A	337	33.830	41.908	67.852	1.00	45.57
	MOTA	2650	N	ARG A	338	34.566	35.733	68.452		25.52
	ATOM	2651	CA	ARG A	338	33.266	35.119	68.508		25.23
	ATOM	2652	c	ARG A		32.944	34.759	69.922		29.77
60	MOTA	2653	ŏ	ARG A		31.854	35.025	70.415		
	ATOM	2654	СВ	ARG A		33.186				31.81
	ATOM	2655	CG				33.920	67.606		24.04
				ARG A		31.839	33.228	67.623		21.31
	ATOM	2656	CD	ARG A		31.807	32.086	66.599		30.62
	MOTA	2657	NE	ARG A	33 5	32.518	30.892	67.040	1.00	29.87

	MOTA	2658	CZ	ARG A	338	31.919	29.781	67.466	1 00	26.37
	ATOM	2659		ARG A		30.616	29.687	67.518		20.26
		2660		ARG A		32.632	28.737	67.864	_	
	ATOM									18.57
_	ATOM	2661	N	HIS A		33.934	34.190	70.577		25.88
5	ATOM	2662	CA	HIS A		33.813	33.797	71.982		25.59
	MOTA	2663	С	HIS A		33.455	34.972	72.892		27.61
	MOTA	2664	0	HIS A		32.615	34.912	73.793	1.00	25.27
	MOTA	2665	CB	HIS A	339	35.065	33.045	72.462		25.06
	ATOM	2666	CG	HIS A	339	34.923	31.587	72.155	1.00	28.13
10	ATOM	2667	ND1	HIS A	339	35.049	30.612	73.127	1.00	30.52
	ATOM	2668	CD2	HIS A	339	34.586	30.970	70.981		30.89
	ATOM	2669	CE1	HIS A	339	34.843	29.442	72.535	1.00	30.89
	ATOM	2670		HIS A		34.546	29.616	71.245		31.36
	ATOM	2671	N	PHE A		34.103	36.065	72.608		24.54
15	ATOM	2672	CA	PHE A		33.892	37.278	73.334		25.36
	ATOM	2673	C	PHE A		32.452	37.762	73.216		32.47
	ATOM	2674	Ö	PHE A		31.822	38.222	74.190		32.78
	ATOM	2675	CB	PHE A		34.876	38.309	72.801		26.03
. ver res.	ATOM	2676	CG	PHE A		34.654	39.671	73.346		26.47
20		2677		PHE A		35.238	40.047	74.559		
Marie Contract of the Contract	MOTA	2678		PHE A	-			72.616		24.59
43	ATOM					33.902	40.592			28.22
h.A.	MOTA	2679		PHE A		35.063	41.330	75.072		21.58
1 at s	ATOM	2680		PHE A		33.715	41.879	73.115		29.13
25	ATOM	2681	CZ	PHE A		34.280	42.225	74.345		25.28
25	MOTA	2682	N	ASN A		31.944	37.663	72.004		28.41
LT.	ATOM	2683	CA.	ASN A		30.600	38.084	71.728		29.60
la fic	ATOM	2684	С	ASN A		29.665	37.110	72.379		38.52
₩	ATOM	2685	0	ASN A		28.699	37.511	73.029		42.88
	MOTA	2686	CB	ASN A		30.322	38.274	70.224		30.01
30	MOTA	2687	CG	ASN A		31.159	39.374	69.587	1.00	52.80
T.i	ATOM	2688		ASN A		31.528	39.284	68.404		60.88
	MOTA	2689		ASN A		31.442	40.427	70.359		41.02
	ATOM	2690	N	ALA A		29.994	35.826	72.239	1.00	28.24
新·明。	ATOM	2691	CA	ALA A		29.195	34.800	72.877	1.00	26.95
35	MOTA	2692	С	ALA A	342	29.013	35.134	74.393	1.00	35.98
En end	MOTA	2693	0	ALA A	342	27.877	35.261	74.897	1.00	35.09
	ATOM	2694	CB	ALA A	342	29.837	33.422	72.671	1.00	25.45
	ATOM	2695	N	LEU A	343	30.153	35.304	75.122	1.00	29.16
	ATOM	2696	CA	LEU A		30.162	35.633	76.560	1.00	22.58
40	ATOM	2697	С	LEU A	343	29.310	36.854	76.831	1.00	27.48
	MOTA	2698	0	LEU A	343	28.452	36.821	77.696	1.00	32.73
	MOTA	2699	CB	LEU A	343	31.583	35.786	77.147	1.00	18.70
	MOTA	2700	CG	LEU A	343	31.647	35.693	78.671	1.00	20.08
	ATOM	2701	CD1	LEU A	343	30.842	34.510	79.204	1.00	17.76
45	ATOM	2702	CD2	LEU A	343	33.091	35.522	79.111	1.00	21.94
	ATOM	2703	N	GLY A		29.512	37.936	76.080	1.00	22.60
	ATOM	2704	CA	GLY A	344	28.670	39.146	76.278	1.00	24.15
	MOTA	2705	С	GLY A	344	27.157	38.824	76.136	1.00	31.38
	MOTA	2706	0	GLY A	344	26.339	39.260	76.943	1.00	32.44
50	ATOM	2707	N	GLY A	345	26.806	38.017	75.094	1.00	22.79
	ATOM	2708	CA	GLY A	345	25.451	37.587	74.801	1.00	19.88
	ATOM	2709	С	GLY A	345	24.787	36.994	76.034	1.00	28.37
	ATOM	2710	0	GLY A	345	23.632	37.294	76.325	1.00	27.56
	ATOM	2711	N	TRP A	346	25.547	36.153	76.765		25.41
55	ATOM	2712	CA.	TRP A	346	25.082	35.520	77.994	1.00	23.90
	MOTA	2713	С	TRP A	346	24.825	36.541	79.071	1.00	31.54
	ATOM	2714	0	TRP A		23.957	36.379	79.924		29.57
	ATOM	2715	CB	TRP A		26.122	34.556	78.562		21.53
	ATOM	2716	CG	TRP A		25.680	33.880	79.837		21.92
60	ATOM	2717		TRP A		25.933	34.335	81.079		24.36
	ATOM	2718		TRP A		25.004	32.597	80.010		20.97
	ATOM	2719		TRP A		25.450	33.453	82.008		23.95
	ATOM	2720		TRP A		24.859	32.388	81.391		24.13
	ATOM	2721		TRP A		24.488	31.611	79.144		21.46

	ATOM	2722	CZ2	TRP A	346	24.225	31.244	81.921	1.00 22.89
	ATOM	2723	CZ3			23.872			
	ATOM	2724	CH2				30.477	79.662	1.00 22.03
	ATOM	2725				23.747	30.286	81.046	1.00 21.87
5			N	GLY A		25.627	37.593	79.039	1.00 29.66
3	ATOM	2726	CA	GLY A		25.465	38.625	80.042	1.00 29.03
	MOTA	2727	С	GLY A		24.156	39.333	79.844	1.00 33.01
	MOTA	2728	0	GLY A	347	23.491	39.647	80.799	1.00 34.17
	MOTA	2729	N	GLU A		23.797	39.574	78.581	
	ATOM	2730	CA	GLU A		22.535			1.00 30.57
10	ATOM	2731	C	GLU A			40.220	78.250	1.00 29.17
. 10						21.423	39.282	78.664	1.00 31.25
	ATOM	2732	0	GLU A		20.373	39.663	79.142	1.00 33.71
	ATOM	2733	CB	GLU A		22.432	40.606	76.757	1.00 30.33
	ATOM	2734	CG	GLU A	348	23.432	41.715	76.336	1.00 49.41
	MOTA	2735	CD	GLU A	348	23.209	43.088	76.964	1.00 73.39
15	ATOM	2736	OE1			22.295	43.846	76.656	
	ATOM	2737	OE2	GLU A	348	24.119	43.395		1.00 71.22
	ATOM	2738	N	LEU A				77.857	1.00 44.23
						21.682	38.011	78.541	1.00 27.36
32 H).	MOTA	2739	CA	LEU A		20.677	37.081	78.976	1.00 26.89
	ATOM	2740	С	LEU A		20.429	37.250	80.485	1.00 24.87
1 20	ATOM	2741	0	LEU A	349	19.299	37.403	80.914	1.00 28.31
42	ATOM	2742	CB	LEU A	349	20.984	35.630	78.529	1.00 27.18
THE SECTION AND ADDRESS OF THE SECTION ADDRESS OF THE S	MOTA	2743	CG	LEU A		19.943	34.565		
p.l.	ATOM	2744		LEU A		18.611		78.942	1.00 32.45
\$ 7 % ====================================	ATOM	2745		LEU A			34.704	78.154	1.00 30.09
25						20.541	33.169	78.749	1.00 27.10
11 4J	ATOM	2746	N	GLN A		21.460	37.255	81.315	1.00 14.78
	ATOM	2747	CA	GLN A		21.188	37.428	82.727	1.00 18.51
∯= €is	MOTA	2748	С	GLN A	350	20.442	38.722	82.953	1.00 25.53
*	ATOM	2749	0	GLN A	350	19.495	38.833	83.737	1.00 28.35
	ATOM	2750	CB	GLN A		22.469	37.369	83.536	
30	ATOM	2751	CG	GLN A		23.512			1.00 22.22
	ATOM	2752	CD	GLN A			36.426	82.919	1.00 22.37
n.						24.871	36.673	83.547	1.00 34.49
1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 -	ATOM	2753		GLN A		25.261	35.932	84.417	1.00 24.01
प्रेय संश् राज्य का	MOTA	2754	NE2	GLN A		25.588	37.727	83.127	1.00 36.58
35	ATOM	2755	N	ASN A		20.838	39.696	82.201	1.00 22.64
L ⊾ 35	ATOM	2756	CA	ASN A	351	20.163	40.960	82.273	1.00 26.10
"	ATOM	2757	С	ASN A		18.661	40.780	82.083	1.00 37.49
	ATOM	2758	0	ASN A		17.890	41.098	82.977	
	ATOM	2759	СВ	ASN A		20.769	42.021		1.00 41.41
	ATOM	2760	CG	ASN A				81.341	1.00 20.74
40	ATOM	2761				22.118	42.477	81.847	1.00 23.25
40				ASN A		22.692	41.875	82 .7 71	1.00 26.88
	MOTA	2762		ASN A		22.644	43.530	81.247	1.00 32.93
	ATOM	2763	N	SER A		18.228	40.252	80.938	1.00 32.84
	ATOM	2764	CA	SER A	352	16.784	40.041	80.715	1.00 34.27
. 12.	MOTA	2765	C	SER A	352	16.107	39.135	81.784	1.00 31.72
45	ATOM	2766	0	SER A	352	14.927	39.266	82.189	1.00 28.64
	ATOM	2767	СВ	SER A		16.503	39.531	79.301	
	ATOM	2768	OG	SER A					1.00 42.57
	ATOM	2769	N	VAL A		17.506	39.979	78.407	1.00 49.17
						16.874	38.188	82.247	1.00 21.90
50	ATOM	2770	CA	VAL A		16.322	37.351	83.234	1.00 22.13
30	MOTA	2771	С	VAL A		16.068	38.122	84.516	1.00 36.22
	MOTA	2772	0	VAL A		14.958	38.076	85.052	1.00 37.69
	ATOM	2773	CB	VAL A	353	17.137	36.070	83.419	1.00 20.84
	ATOM	2774	CG1	VAL A	353	16.632	35.256	84.634	1.00 15.06
	ATOM	2775		VAL A		16.968	35.284		
55	ATOM	2776	N	LYS A				82.105	1.00 20.93
						17.086	38.847	85.002	1.00 30.67
	ATOM	2777	CA	LYS A		16.880	39.587	86.221	1.00 31.71
	ATOM	2778	C	LYS A		15.660	40.474	86.098	1.00 36.17
	ATOM	2779	0	LYS A		14.808	40.582	86.980	1.00 35.80
	MOTA	2780	CB	LYS A		18.099	40.396	86.624	1.00 35.28
60	ATOM	2781	CG	LYS A		17.841	41.303	87.818	
	ATOM	2782	CD	LYS A		19.038	41.405		1.00 51.51
	ATOM	2783	CE	LYS A				88.749	1.00 60.46
	ATOM	2784	NZ			19.198	42.780	89.383	1.00 50.09
	ATOM			LYS A			43.133	89.657	1.00 63.77
	ATOM	2785	N	THR A	3,33	15.608	41.108	84.962	1.00 32.63
	and the second second								

		MOTA	2786	CA	THR A	355	14.562	42.025	84.610	1.00 34.03
		ATOM	2787	С	THR A	355	13.129	41.422	84.578	1.00 42.11
		ATOM	2788	0	THR A	355	12.216	42.006	85.154	1.00 40.96
		ATOM	2789	CB	THR A		14.974	42.736	83.308	1.00 41.11
	5	ATOM	2790		THR A		16.071	43.615	83.542	1.00 29.85
		MOTA	2791		THR A		13.798	43.438	82.656	1.00 45.50
		MOTA	2792	N	PHE A		12.895	40.273	83.908	1.00 33.89
				CA	PHE A			39.729	83.860	1.00 33.09
		MOTA	2793				11.556			
	10	ATOM	2794	C	PHE A		11.209	39.070	85.147	1.00 31.93
	10	MOTA	2795	0	PHE A		10.089	39.152	85.642	1.00 33.85
		ATOM	2796	CB	PHE A		11.460	38.645	82.785	1.00 33.30
		ATOM	2797	CG	PHE A		11.187	39.196	81.416	1.00 36.54
		MOTA	2798		PHE A		10.106	40.054	81.224	1.00 42.38
		MOTA	2799	CD2	PHE A	356	11.985	38.858	80.320	1.00 38.62
	15	MOTA	2800	CE1	PHE A	356	9.831	40.596	79.968	1.00 44.75
		ATOM	2801	CE2	PHE A	356	11.723	39.384	79.055	1.00 43.46
		ATOM	2802	CZ	PHE A	356	10.649	40.261	78.890	1.00 43.86
		ATOM	2803	N	GLY A		12.212	38.386	85.661	1.00 30.41
## ₉		ATOM	2804	CA	GLY A		12.152	37.564	86.864	1.00 29.17
şaπiş ≎aπiş	20	MOTA	2805	C	GLY A		12.446	36.100	86.438	1.00 28.92
See Mary	20		2806		GLY A					1.00 20.32
uil.		MOTA		0			12.008	35.642	85.372	
hada		ATOM	2807	N	GLU A		13.211	35.382	87.243	1.00 21.27
12 H/2 2 H/2		ATOM	2808	CA	GLU A		13.590	34.040	86.898	1.00 23.10
3 247 112 247		MOTA	2809	С	GLU A		12.424	33.104	86.747	1.00 31.53
3 77 k	25	ATOM	2810	0	GLU A		12.581	31.972	86.294	1.00 30.92
LT.		MOTA	2811	CB	GLU A	358	14.596	33.473	87.880	1.00 25.36
partie.		ATOM	2812	CG	GLU A	358	14.011	33.436	89.301	1.00 38.73
		ATOM	2813	CD	GLU A	358	15.011	33.037	90.345	1.00 56.34
#E		ATOM	2814	OE1	GLU A	358	16.026	32.446	90.071	1.00 50.55
	30	ATOM	2815		GLU A		14.678	33.403	91.564	1.00 75.65
T,	-	ATOM	2816	N	THR A		11.246	33.542	87.139	1.00 27.87
		ATOM	2817	CA	THR A		10.154	32.625	86.970	1.00 25.66
		ATOM	2818	C	THR A		9.236	33.152	85.906	1.00 25.96
va al∉			2819	Ö	THR A		8.247	32.528	85.533	1.00 25.58
in and	35	MOTA								
1=Bo	33	ATOM	2820	CB	THR A		9.423	32.341	88.253	1.00 25.00
		ATOM	2821		THR A		8.908	33.565	88.692	1.00 33.10
		ATOM	2822		THR A		10.406	31.785	89.273	1.00 14.43
		ATOM	2823	N	HIS A		9.602	34.310	85.407	1.00 20.75
	40	ATOM	2824	CA	HIS A		8.837	34.902	84.363	1.00 22.77
	40	ATOM	2825	С	HIS A		8.823	34.034	83.130	1.00 35.30
		MOTA	2826	0	HIS A	360	9.858	33.611	82.620	1.00 37.42
		MOTA	2827	CB	HIS A	360	9.294	36.291	83.982	1.00 23.18
		ATOM	2828	CG	HIS A	360	8.207	36.908	83.219	1.00 27.05
		ATOM	2829	ND1	HIS A	360	7.532	38.009	83.691	1.00 29.34
	45	ATOM	2830	CD2	HIS A	360	7.651	36.545	82.059	1.00 29.91
		MOTA	2831	CE1	HIS A	360	6.596	38.315	82.806	1.00 27.94
		MOTA	2832		HIS A		6.651	37.440	81.812	1.00 29.60
		MOTA	2833	N	PRO A		7.606	33.817	82.666	1.00 32.40
		ATOM	2834	CA	PRO A		7.301	32.999	81.519	1.00 29.46
	50	ATOM	2835	C	PRO A		7.862	33.478	80.224	1.00 30.59
	-	ATOM	2836	Õ	PRO A		7.907	32.737	79.248	1.00 33.00
		ATOM	2837	СВ	PRO A		5.770	32.963	81.478	1.00 33.00
		ATOM	2838	CG	PRO A		5.311	33.172	82.927	1.00 34.96
	55	ATOM	2839	CD	PRO A		6.463	33.869	83.627	1.00 31.82
	55	MOTA	2840	N	PHE A		8.289	34.712	80.179	1.00 26.32
		MOTA	2841	CA	PHE A		8.823	35.173	78.933	1.00 25.68
		MOTA	2842	C	PHE A		10.261	34.781	78.829	1.00 29.73
		ATOM	2843	0	PHE A		10.906	35.131	77.870	1.00 32.02
		ATOM	2844	CB	PHE A	362	8.643	36.677	78.723	1.00 28.12
	60	ATOM	2845	CG	PHE A	362	7.194	37.105	78.629	1.00 30.03
		MOTA	2846	CD1	PHE A	362	6.204	36.276	78.098	1.00 30.92
		MOTA	2847		PHE A		6.804	38.372	79.051	1.00 32.04
		ATOM	2848	CE1	PHE A	362	4.864	36.655	77.998	1.00 26.59
		ATOM	2849		PHE A		5.470	38.773	78.952	1.00 32.40
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	ATOM	2914	С	ASP A	271	-2.557	37.636	75.255	1.00 40.92
	MOTA	2915	0	ASP A		-2.784	38.625	75.933	1.00 41.63
	MOTA	2916	CB	ASP A		-4.519	36.375	76.245	1.00 39.88
	MOTA	2917	CG	ASP A	371	-5.805	35.733	75.798	1.00 51.30
5	MOTA	2918	OD1	ASP A	371	-6.373	36.072	74.761	1.00 50.39
.=	ATOM	2919	OD2	ASP A	371	-6.206	34.754	76.583	1.00 48.61
	ATOM	2920	N	ILE A		-1.387	37.398	74.664	1.00 36.37
	ATOM	2921	CA	ILE A		-0.259	38.283	74.817	1.00 34.61
	MOTA	2922	С	ILE A		0.203	39.018	73.555	1.00 35.46
10	MOTA	2923	0	ILE A	372	0.545	38.400	72.548	1.00 36.69
	ATOM	2924	CB	ILE A	372	0.920	37.511	75.381	1.00 36.51
	ATOM	2925		ILE A		0.658	37.195	76.842	1.00 37.01
	MOTA	2926	CG2	ILE A		2.121	38.441	75.281	1.00 35.52
	MOTA	2927	CD1	ILE A	372	1.268	38.261	77.747	1.00 54.33
15	ATOM	2928	N	ASP A	373	0.254	40.345	73.601	1.00 25.92
	ATOM	2929	CA	ASP A	373	0.747	41.053	72.450	1.00 23.77
	ATOM	2930	C	ASP A		2.263	40.781	72.360	1.00 31.40
	ATOM	2931	0	ASP A		3.040	41.002	73.305	1.00 32.80
	ATOM	2932	CB	ASP A		0.408	42.543	72.519	1.00 25.08
20	ATOM	2933	CG	ASP A	. 373	1.064	43.356	71.418	1.00 43.24
	MOTA	2934	OD1	ASP A	373	1.861	42.894	70.616	1.00 45.30
	ATOM	2935		ASP A		0.668	44.610	71.395	1.00 38.59
	MOTA	2936	N	PRO A		2.709	40.267	71.225	1.00 29.51
	MOTA	2937	CA	PRO A		4.123	39.943	71.132	1.00 28.52
25	ATOM	2938	С	PRO A	374	5.029	41.090	71.506	1.00 32.54
	ATOM	2939	0	PRO A	374	6.019	40.905	72.217	1.00 29.62
	ATOM	2940	CB	PRO A		4.390	39.421	69.714	1.00 28.88
	MOTA	2941	CG	PRO A		3.028	39.278	69.032	1.00 20.00
20	ATOM	2942	CD	PRO A		1.966	39.786	70.008	1.00 28.84
30	ATOM	2943	N	ASP A	. 375	4.660	42.257	70.981	1.00 26.85
	ATOM	2944	CA	ASP A	375	5.357	43.511	71.154	1.00 24.25
	ATOM	2945	С	ASP A	375	5.695	43.783	72.628	1.00 33.10
	ATOM	2946	0	ASP A		6.648	44.494	72.988	1.00 30.67
		2947	СВ	ASP A		4.507	44.617	70.509	1.00 30.07
25	MOTA								
35	MOTA	2948	CG	ASP A		4.753	44.836	69.033	1.00 30.08
	ATOM	2949	OD1	ASP A	375	5.703	44.393	68.411	1.00 33.47
	ATOM	2950	OD2	ASP A	375	3.852	45.609	68.491	1.00 38.41
	ATOM	2951	N	VAL A	376	4.885	43.161	73.477	1.00 30.21
	ATOM	2952	CA	VAL A		5.001	43.232	74.904	1.00 25.40
40		2953		VAL A		5.879	42.106	75.431	1.00 23.40
40	ATOM		C						
	MOTA	2954	0	VAL A		6.599	42.299	76.394	1.00 42.46
	ATOM	2955	CB	VAL A	376	3.638	43.099	75.550	1.00 22.48
	ATOM	2956	CG1	VAL A	376	3.799	42.533	76.975	1.00 21.25
	ATOM	2957	CG2	VAL A	376	2.926	44.440	75.547	1.00 18.29
45	ATOM	2958	N	ALA A		5.811	40.905	74.831	1.00 30.48
	ATOM	2959	CA	ALA A		6.671	39.793	75,288	
									1.00 27.04
	ATOM	2960	С	ALA A		8.149	39.911	74.797	1.00 28.15
	ATOM	2961	0	ALA A	377	9.077	39.325	75.312	1.00 27.36
	ATOM	2962	CB	ALA A	377	6.091	38.433	74.891	1.00 26.74
50	ATOM	2963	N	TYR A		8.376	40.692	73.768	1.00 25.81
	ATOM	2964	CA	TYR A		9.683	40.876	73.161	1.00 25.43
	MOTA	2965	C	TYR A		10.862	41.194	74.057	1.00 30.49
	MOTA	2966	0	TYR A		10.873	42.204	74.747	1.00 32.35
	MOTA	2967	CB	TYR A	A 378	9.549	41.924	72.068	1.00 26.20
55	ATOM	2968	CG	TYR A	378	10.804	42.168	71.327	1.00 19.90
	ATOM	2969		TYR A		11.256	41.231	70.406	1.00 18.53
		2970					43.331		1.00 18.47
	ATOM			TYR A		11.536		71.543	
	ATOM	2971		TYR A		12.444	41.436	69.716	1.00 15.98
	MOTA	2972	CE2	TYR A	A 378	12.719	43.555	70.840	1.00 18.77
60	ATOM	2973	CZ	TYR A	A 378	13.161	42.609	69.920	1.00 16.37
	ATOM	2974	OH	TYR F		14.309	42.811	69.212	1.00 32.30
	ATOM	2975	N.	SER A		11.879	40.317	73.977	1.00 23.03
	ATOM	2976	CA	SER A		13.115	40.430	74.725	1.00 18.13
	MOTA	2977	С	SER A	a 379	14.267	39.777	73.970	1.00 20.60

			ATOM	2850	CZ	PHE A	362	4.495	37.920	78.435	1.00 26.37
			ATOM	2851	N	THR A	363	10.730	34.049	79.843	1.00 27.22
			ATOM	2852	CA	THR A		12.102	33.575	79.943	1.00 27.52
			ATOM	2853	С	THR A	363	12.251	32.132	79.504	1.00 29.28
	5		MOTA	2854	0	THR A	363	13.331	31.560	79.524	1.00 29.42
			ATOM	2855	CB	THR A	363	12.697	33.777	81.360	1.00 31.67
			ATOM	2856	OG1	THR A	363	12.279	32.745	82.218	1.00 26.17
			MOTA	2857	CG2	THR A	363	12.278	35.118	81.930	1.00 31.62
			ATOM	2858	N	LYS A	364	11.148	31.530	79.113	1.00 23.08
	10		ATOM	2859	CA	LYS A		11.174	30.160	78.664	1.00 20.50
			MOTA	2860	С	LYS A		11.556	30.270	77.217	1.00 28.83
			MOTA	2861	0	LYS A		11.139	31.239	76.570	1.00 29.80
			MOTA	2862	CB	LYS A		9.766	29.584	78.667	1.00 23.55
	1.5		ATOM	2863	CG	LYS A		9.252	29.134	80.022	1.00 40.85
	15		ATOM	2864	CD	LYS A		7.761	29.369	80.162	1.00 44.83
	`		MOTA	2865	CE	LYS A		7.131	28.492	81.224	1.00 66.38
			ATOM	2866	NZ	LYS A		6.063	27.638	80.691	1.00 91.70
Sep. 10.		•	ATOM	28 67 2868	N CA	LEU A		12.332	29.328	76.698	1.00 23.57
	20		ATOM ATOM	2869	C	LEU A		12.699 11.414	29.420 29.419	75.312	1.00 23.95
	20		ATOM	2870	Ö	LEU A		11.166	30.369	74.445	1.00 35.57
The state of the s			ATOM	2871	CB	LEU A		13.702	28.303	73.708 75.021	1.00 34.58
ga ik			ATOM	2872	CG	LEU A		14.456	28.372	73.702	1.00 25.08 1.00 31.15
सर्वे स्थाः इसः	•		ATOM	2873		LEU A		14.987	29,778	73.466	1.00 31.15
THE THE PERSON NAMED IN COLUMN TWO IS NOT THE PERSON NAMED IN COLUMN T	25		ATOM	2874		LEU A		15.609	27.353	73.781	1.00 33.16
L THE			ATOM	2875	N	VAL A		10.572	28.360	74.564	1.00 35.62
E=Ex			ATOM	2876	CA	VAL A		9.294	28.232	73.840	1.00 33.02
學			ATOM	2877	С	VAL A		8.211	28.911	74.694	1.00 33.14
			ATOM	2878	0	VAL A		7.982	28.470	75.808	1.00 34.20
þá. F	30		MOTA	2879	CB	VAL A		8.936	26.739	73.568	1.00 34.73
n.			ATOM	2880	CG1	VAL A		7.558	26.605	72.933	1.00 34.88
			MOTA	2881	CG2	VAL A	366	9.922	26.012	72.649	1.00 32.65
12.11			ATOM	2882	N	VAL A	367	7.562	29.990	74.211	1.00 28.76
(an)	~ =		ATOM	2883	CA	VAL A		6.532	30.700	74.987	1.00 28.27
]=	35		MOTA	2884	С	VAL A		5.161	30.613	74.420	1.00 30.62
			ATOM	2885	0	VAL A		4.994	30.509	73.235	`1.00 34.30
			ATOM	2886	СВ	VAL A		6.773	32.185	75.061	1.00 33.45
			ATOM	2887		VAL A		8.178	32.478	75.565	1.00 33.03
	40		ATOM ATOM	2888 2889	N	VAL A		6.498	32.804	73.693	1.00 33.18
	-10		ATOM	2890	CA	ASP A		4.168 2.764	30.722 30.771	75.290 74.984	1.00 29.27 1.00 27.67
			ATOM	2891	C	ASP A		2.315	32.207	74.862	1.00 27.07
			ATOM	2892	ŏ	ASP A		2.283	32.975	75.830	1.00 20.34
			MOTA	2893	CB	ASP A		1.990	30.073	76.100	1.00 26.80
	45		ATOM	2894	CG	ASP A		0.572	29.781	75.613	1.00 37.90
			MOTA	2895	OD1	ASP A		0.276	30.123	74.481	1.00 38.93
			ATOM	2896		ASP A		-0.215	29.217	76.380	1.00 38.59
			ATOM	2897	N	LEU A	369	2.027	32.588	73.622	1.00 26.55
	~^		MOTA	2898	CA	LEU A		1.643	33.953	73.373	1.00 27.39
	50		ATOM	2899	С	LEU A		0.138	34.105	73.301	1.00 30.74
			ATOM	2900	0	LEU A		-0.372	34.979	72.648	1.00 30.68
			ATOM	2901	CB	LEU A		2.281	34.395	72.064	1.00 26.06
. 7			ATOM	2902	CG	LEU A		3.759	34.760	72.229	1.00 26.80
	55		ATOM	2903		LEU A		4.343	35.415	70.994	1.00 24.30
	55		ATOM	2904		LEU A		4.014	35.728	73.384	1.00 21.81
			ATOM	2905	N CA	THR A		-0.577	33.154	73.953	1.00 30.26
			MOTA MOTA	2906	CA C	THR A		-2.022	33.306	74.093	1.00 31.38
			ATOM	2907 2908	0	THR A		-2.355	34.519	74.941	1.00 38.62
	60		ATOM	2909	СВ	THR A		-1.821 -2.601	34.714 32.056	76.027 74.750	1.00 38.84 1.00 34.04
			ATOM	2910		THR A		-2.472	30.949	73.873	1.00 34.04
			ATOM	2911		THR A		-4.091	32.266	75.052	1.00 29.99
			ATOM	2912	N	ASP A		-3.173	35.387	74.363	1.00 20.40
			ATOM	2913	CA	ASP A		-3.641	36.612	75.012	1.00 37.85
											27.03

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	ATOM	2978	0	SER A	379	14.100	39.334	72.843	1.00 18.46
	ATOM	2979	СВ	SER A		12.976	39.740	76.067	1.00 23.56
	ATOM	2980	OG	SER A	379	12.805	38.329	75.883	1.00 37.26
	MOTA	2981	N	SER A	380	15.424	39.697	74.651	1.00 23.65
5	ATOM	2982	CA	SER A	380	16.701	39.084	74.222	1.00 26.09
	MOTA	2983	С	SER A	380	16.669	37.571	74.457	1.00 28.37
	ATOM	2984	0	SER A	380	17.480	36.785	73.975	1.00 30.81
	MOTA	2985	CB	SER A		17.889	39.588	75.062	1.00 31.60
	ATOM	2986	OG	SER A	380	18.036	41.000	75.033	1.00 42.48
10	MOTA	2987	N	VAL A		15.718	37.188	75.260	1.00 18.04
	ATOM	2988	CA	VAL A		15.595	35.812	75.598	1.00 14.91
	ATOM	2989	С	VAL A		15.708	34.897	74.419	1.00 20.31
	MOTA	2990	0	VAL A		16.620	34.091	74.330	1.00 27.64
16	MOTA	2991	CB	VAL A		14.408	35.546	76.501	1.00 16.34
15	ATOM	2992		VAL A		14.284	34.062	76.734	1.00 17.26
	MOTA	2993		VAL A		14.687	36.204	77.829	1.00 13.94
	MOTA	2994	N	PRO A		14.797	35.005	73.489	1.00 16.53
	ATOM	2995	CA	PRO A		14.886	34.139	72.324	1.00 17.21
20	ATOM	2996	C	PRO A		16.222	34.230	71.634	1.00 24.01
20	ATOM	2997 2998	O CB	PRO A		16.709 13.777	33.192	71.207	1.00 27.79
	ATOM ATOM	2999	CG	PRO A		13.003	34.514 35.618	71.351 72.033	1.00 17.20
	ATOM	3000	CD	PRO A		13.627	35.873	73.399	1.00 18.32 1.00 12.12
	ATOM	3001	N	TYR A		16.809	35.447	71.542	1.00 12.12
25	MOTA	3002	CA	TYR A		18.112	35.648	70.902	1.00 19.33
20	ATOM	3003	c	TYR A		19.246	34.953	71.651	1.00 28.79
	ATOM	3004	ō	TYR A		19.980	34.117	71.104	1.00 31.38
	ATOM	3005	CB	TYR A		18.468	37.135	70.894	1.00 21.02
	ATOM	3006	CG	TYR A		17.593	37.968	70.011	1.00 23.86
30	ATOM	3007	CD1	TYR A	383	16.290	38.277	70.404	1.00 28.36
	ATOM	3008	CD2	TYR A	383	18.067	38.450	68.784	1.00 20.93
	MOTA	3009	CE1	TYR A	383	15.473	39.054	69.576	1.00 30.88
	MOTA	3010	CE2	TYR A	383	17.272	39.244	67.957	1.00 18.71
	ATOM	3011	CZ	TYR A		15.967	39.533	68.358	1.00 25.95
35	ATOM	3012	OH	TYR A		15.171	40.294	67.556	1.00 30.84
	MOTA	3013	N	GLU A		19.389	35.333	72.921	1.00 20.17
	ATOM	3014	CA	GLU A		20.419	34.857	73.803	1.00 17.57
	ATOM	3015	C	GLU A		20.188	33.506	74.405	1.00 22.88
40	ATOM	3016	0	GLU A		21.151	32.775	74.669	1.00 25.65
. 40	MOTA	3017	CB	GLU A		20.833	35.973	74.773	1.00 20.44
	ATOM	3018	CG CD	GLU A		21.263	37.202	73.944	1.00 15.21
	ATOM ATOM	3019 3020		GLU A		22.539 23.185	36.937 35.915	73.184 73.293	1.00 26.58 1.00 17.84
	ATOM	3021		GLU A		22.887	37.915	72.400	1.00 17.84
45	ATOM	3022	N	LYS A		18.935	33.116	74.610	1.00 20.33
•••	ATOM	3023	CA	LYS A		18.736	31.767	75.146	1.00 20.05
	ATOM	3024	С	LYS A		18.865	30.716	74.028	1.00 27.19
	ATOM	3025	0	LYS A		19.420	29.621	74.219	1.00 31.66
	MOTA	3026	CB	LYS A		17.507	31.577	76.014	1.00 21.51
50	ATOM	3027	CG	LYS A	385	17.676	30.384	76.953	1.00 22.29
	ATOM	3028	CD	LYS A	385	16.386	29.820	77.518	1.00 19.87
	MOTA	3029	CE	LYS A		16.049	30.277	78.937	1.00 31.60
	ATOM	3030	NZ	LYS A		14.783	29.694	79.441	1.00 30.38
	ATOM	3031	N	GLY A		18.364	31.084	72.832	1.00 20.72
55	MOTA	3032	CA	GLY A		18.453	30.248	71.637	1.00 17.41
	ATOM	3033	С	GLY A		19.924	30.106	71.298	1.00 20.81
	ATOM	3034	0	GLY A		20.396	29.001	71.225	1.00 22.50
	ATOM	3035	N	PHE A		20.683	31.228	71.163	1.00 20.30
60	MOTA	3036	CA	PHE A		22.137	31.158	70.900	1.00 19.92
60	MOTA	3037	С	PHE A		22.840	30.263	71.905	1.00 29.09
	ATOM	3038	O	PHE A		23.685	29.478	71.530	1.00 32.80
	MOTA MOTA	3039 3040	CB CG	PHE A		22.852 24.344	32.519 32.358	70.955 70.872	1.00 20.07 1.00 19.41
	ATOM	3041		PHE A		24.949	32.163	69.631	1.00 19.41
							52.105	.00.001	2.00 23.01
							4.		

		ATOM	3042	CD2	PHE A	387	25.157	32.373	72.007	1.00 25.27
		MOTA	3043		PHE A		26.329	31.977	69.525	1.00 20.88
		ATOM	3044	CE2	PHE A	387	26.542	32.202	71.916	1.00 28.83
		ATOM	3045	CZ	PHE A	387	27.131	31.981	70.668	1.00 23.24
	5				ALA A		22.495	30.381	73.203	1.00 25.48
)	MOTA	3046	N						
		ATOM	3047	CA	ALA A	388	23.133	29.556	74.242	1.00 23.14
		ATOM	3048	С	ALA A	388.	22.872	28.108	74.055	1.00 32.10
		MOTA	3049	0	ALA A	388	23.757	27.282	74.258	1.00 37.82
		ATOM	3050	CB	ALA A	388	22.717	29.932	75.633	1.00 23.02
	10		3051	N .	LEU A		21.636	27.793	73.691	
	IV	MOTA								1.00 26.31
		ATOM	3052	CA	LEU A	389	21.275	26.405	73.460	1.00 21.42
		ATOM	3053	С	LEU A	389	22.189	25.906	72.372	1.00 27.91
		MOTA	3054	0	LEU A	389	22.865	24.900	72.532	1.00 29.25
		MOTA	3055	CB	LEU A	389	19.841	26.300	72.937	1.00 19.24
	15	MOTA	3056	CG	LEU A	380	19.427	24.868	72.632	1.00 17.17
	1.5									
		MOTA	3057		LEU A		19.717	24.017	73.844	1.00 14.63
		ATOM	3058	CD2	LEU A	389	17.943	24.808	72.328	1.00 10.16
			3059	N	LEU A		22.217	26.659		
.622.000.		ATOM							71.262	1.00 24.49
ian.		MOTA	3060	CA	LEU A	390	23.050	26.340	70.107	1.00 25.05
LD	20	MOTA	3061	С	LEU A	390	24.531	26.256	70,383	1.00 32.31
reduction.										
wij)		ATOM	3062	0	LEU A		25.183	25.301	69.932	1.00 33.60
ļ=ā.		ATOM	3063	CB	LEU A	390	22.765	27.152	68.844	1.00 23.33
		ATOM	3064	CG	LEU A		21.307	27.026	68.442	1.00 23.38
100 mg mg 100 mg										
2 240	1 1	ATOM	3065	CD1	LEU A	390	20.986	28.025	67.334	1.00 20.84
(#####################################	25	ATOM	3066	CD2	LEU A	390	20.988	25.591	68.017	1.00 18.86
LT.			3067		PHE A		25.058	27.231		
		ATOM		N					71.127	1.00 28.52
1 - A		ATOM	3068	CA	PHE A	391	26.480	27.236	71.494	1.00 27.82
		ATOM	3069	С	PHE A	391	26.813	25.992	72.312	1.00 28.67
hada.	•	ATOM	3070	0	PHE A		27.839	25.331	72.148	1.00 26.96
	30	MOTA	3071	CB	PHE A	391	26.834	28.455	72.341	1.00 28.60
f.		ATOM	3072	CG	PHE A	301	28.296	28.786	72.283	1.00 30.53
n.										
11 1924		MOTA	3073		PHE A		28.967	28.816	71.064	1.00 35.08
		MOTA	3074	CD2	PHE A	391	29.020	29.063	73.440	1.00 36.52
		MOTA	3075		PHE A		30.320	29.142	70.983	
	26									1.00 37.61
-4	35	MOTA	3076	CE2	PHE A	391	30.378	29.383	73.382	1.00 40.61
	. •	ATOM	3077	CZ	PHE A	391	31.026	29.432	72.148	1.00 37.64
			3078							
		MOTA		N	TYR A		25.913	25.699	73.225	1.00 24.90
		ATOM	3079	CA	TYR A	392	26.044	24.550	74.065	1.00 24.66
		ATOM	3080	С	TYR A	392	26.106	23.298	73.186	1.00 34.30
	40									
	40	ATOM	3081	0	TYR A		27.058	22.558	73.268	1.00 37.51
		ATOM	3082	CB	TYR A	392	24.821	24.501	74.967	1.00 26.39
		ATOM	3083	CG	TYR A	392	24.631	23.181	75.678	1.00 31.99
		ATOM	3084	CD1	TYR A		25.546	22.715	76.625	1.00 35.17
		MOTA	3085	CD2	TYR A	392	23.501	22.397	75.432	1.00 32.49
	45	ATOM	3086	CEI	TYR A	392	25.341	21.512	77.306	
										1.00 39.01
		ATOM	3087		TYR A		23.281	21.184	76.094	1.00 31.50
		ATOM	3088	CZ	TYR A	392	24.206	20.743	77.035	1.00 34.08
		ATOM	3089	OH	TYR A		23.986	19.564	77.683	1.00 36.46
		MOTA	3090	N	LEU A		25.101	23.067	72.310	1.00 31.02
	50	MOTA	3091	CA	LEU A	393	25.043	21.889	71.410	1.00 29.65
		MOTA	3092	С	LEU A	२०२	26.274	21.616	70.507	1.00 32.03
		MOTA	3093	0	LEU A		26.664	20.468	70.267	1.00 27.90
		ATOM	3094	CB	LEU A	393	23.758	21.905	70.552	1.00 28.85
		ATOM	3095	CG	LEU A		22.489	21.688	71.375	
	22									1.00 30.33
	55	MOTA	3096		LEU A		21.256	22.047	70.559	1.00 27.38
		ATOM	3097	CD2	LEU A	393	22.400	20.246	71.865	1.00 29.76
		MOTA	3098	N	GLU A		26.841	22.701	69.980	1.00 30.84
	7	ATOM	3099	CA	GLU A	394	28.000	22.727	69.118	1.00 30.05
		ATOM	3100	С	GLU A		29.210	22.214	69.868	1.00 39.16
	60									
	50	MOTA	3101	0	GLU A		30.089	21.595	69.299	1.00 42.14
		MOTA	3102	CB	GLU A	394	28.300	24.204	68.756	1.00 31.03
		ATOM	3103	CG	GLU A		29.776	24.406	68.376	1.00 37.11
		ATOM	3104	CD	GLU A		30.182	25.830	68.208	1.00 45.20
		ATOM	3105	OE1	GLU A	394	29.614	26.609	67.471	1.00 56.77
7.5										

		ATOM	3106	OE2	GLU A	394	31.229	26.133	68.927	1.00 39.77
		ATOM	3107		GLN A		29.256	22.534	71.160	1.00 34.20
		ATOM	3108		GLN A		30.342	22.139	72.029	1.00 32.86
		ATOM	3109		GLN A		30.143	20.690	72.435	1.00 32.65
	5		3110		GLN A		31.066	19.899	72.507	1.00 38.67
	3	ATOM	3111		GLN A		30.474	23.051	73.287	1.00 33.17
		MOTA								
		ATOM	3112		GLN A		30.831	24.540	72.996	1.00 13.79
		MOTA	3113		GLN A		31.176	25.354	74.247	1.00 37.45
	10	ATOM	3114		GLN A		30.909	24.959	75.407	1.00 26.89
	10	ATOM	3115		GLN A		31.758	26.523	74.010	1.00 31.99
		MOTA	3116		LEU A		28.903	20.352	72.682	1.00 38.68
		MOTA	3117		LEU A		28.514	19.015	73.083	1.00 38.49
	3 March 19	MOTA	3118	С	LEU A	396	28.633	18.017	71.924	1.00 39.28
		MOTA	3119		LEU A		29.012	16.871	72.100	1.00 42.17
	15	MOTA	3120	CB	LEU A	396	27.055	19.072	73.628	1.00 37.93
		ATOM	3121	CG	LEU A	396	26.389	17.732	73.946	1.00 42.72
* .		ATOM	3122	CD1	LEU A	396	26.436	17.489	75.445	1.00 45.42
		ATOM	3123		LEU A		24.917	17.709	73.527	1.00 43.81
		ATOM	3124		LEU A		28.303	18.456	70.730	1.00 28.48
	20	ATOM	3125		LEU A		28.337	17.595	69.589	1.00 25.49
THE ENT	20	MOTA	3126		LEU A		29.620	17.609	68.771	1.00 36.86
W.			3127		LEU A		29.596	17.220	67.599	1.00 30.85
ļ.Ł.		ATOM			LEU A		27.156	17.220		
		ATOM	3128						68.686	1.00 23.73
	25	ATOM	3129	CG	LEU A		25.843	17.773	69.401	1.00 25.82
I Fig.	25	MOTA	3130		LEU A		24.740	18.559	68.669	1.00 22.99
% a €		ATOM	3131		LEU A		25.525	16.272	69.452	1.00 27.30
ļub,		MOTA	3132	N	GLY A		30.731	18.069	69.342	1.00 33.98
**		MOTA	3133	CA	GLY A		31.993	18.038	68.617	1.00 34.14
Jada	•	MOTA	3134	С	GLY A		32.547	19.260	67.889	1.00 38.92
T.	30	ATOM	3135	0	GLY A		33.502	19.097	67.115	1.00 39.98
		ATOM	3136	N	GLY A		32.001	20.457	68.105	1.00 33.01
		ATOM	3137	CA	GLY A	399	32.543	21.650	67.440	1.00 30.35
		MOTA	3138	С	GLY A	399	31.713	22.336	66.365	1.00 31.72
20 Mg		MOTA	3139	0	GLY A	399	30.800	21.823	65.762	1.00 34.57
	35	ATOM	3140	N	PRO A	400	32.076	23.550	66.124	1.00 33.01
4		ATOM	3141	CA	PRO A	400	31.429	24.406	65.151	1.00 35.02
		ATOM	3142	С	PRO A		31.379	23.794	63.750	1.00 43.93
		ATOM	3143	0	PRO A	400	30.360	23.838	63.045	1.00 40.14
		ATOM	3144	СВ	PRO A	400	32.293	25.672	65.111	1.00 35.73
	40	ATOM	3145	CG	PRO A		33.539	25,411	65.948	1.00 38.03
	••	ATOM	3146	CD	PRO A		33.423	24.010	66.517	1.00 33.92
		ATOM	3147	N	GLU A		32.512	23.237	63.345	1.00 43.85
		ATOM	3148	CA	GLU A		32.597	22.620	62.042	1.00 42.92
		ATOM	3149	C	GLU A		31.491	21.587	61.878	1.00 37.92
	45	ATOM	3150	ő	GLU A		30.810	21.588	60.866	1.00 33.79
		ATOM	3151	СВ	GLU A		33.996	22.034	61.789	1.00 45.93
		ATOM	3152	CG	GLU A		34.578	22.372	60.398	1.00 69.62
		MOTA	3153	CD	GLU A		35.603	21.373	59.911	1.00100.00
							36.702		60.427	
	50	ATOM	3154		GLU A			21.236		1.00100.00
	50	ATOM	3155		GLU A		35.195	20.689	58.865	1.00 93.16
		ATOM	3156	N	ILE A		31.317	20.720	62.902	1.00 34.58
		ATOM	3157	CA	ILE A		30.281	19.681	62.922	1.00 33.20
		ATOM	3158	C	ILE A		28.898	20.291	62.938	1.00 39.09
	EE	ATOM	3159	0	ILE A		28.065	19.896	62.133	1.00 41.43
	55	ATOM	3160	CB	ILE A		30.391	18.673	64.078	1.00 33.82
		MOTA	3161		ILE A		31.490	17.661	63.811	1.00 34.70
		ATOM	3162		ILE A		29.080	17.900	64.287	1.00 23.32
		ATOM	3163		ILE A		31.878	16.896	65.080	1.00 49.20
		ATOM	3164	N	PHE A		28.668	21.246	63.868	1.00 32.73
	60	ATOM	3165	CA	PHE A	403	27.390	21.952	64.044	1.00 29.52
		ATOM	3166	С	PHE A	403	27.032	22.816	62.836	1.00 33.94
		MOTA	3167	0	PHE A	403	25.866	23.022	62.469	1.00 34.15
		MOTA	3168	CB	PHE A		27.319	22.719	65.381	1.00 29.03
		ATOM	3169	CG	PHE A		25.917	22.783	65.929	1.00 28.54

		0150	an 1			05 000			
	MOTA	3170		PHE A		25.323	21.643	66.484	1.00 29.91
	MOTA	3171	CD2	PHE A	403	25.176	23.964	65.873	1.00 27.62
	MOTA	3172	CE1	PHE A	403	24.021	21.667	66.990	1.00 27.38
	ATOM	3173	CE2	PHE A	403	23.881	24.017	66.393	1.00 28.82
5		3174	CZ	PHE A					
, ,	ATOM					23.304	22.863	66.932	1.00 25.72
	ATOM	3175	N	LEU A		28.040	23.327	62.165	1.00 31.31
	ATOM	3176	CA	LEU A	404	27.687	24.080	60.983	1.00 32.95
	ATOM	3177	С	LEU A	404	27.068	23.099	59.952	1.00 32.89
	ATOM	3178	0	LEU A		26.050	23.361	59.315	1.00 37.36
10									
10	ATOM	3179	CB	LEU A		28.798	25.045	60.464	1.00 33.15
	ATOM	3180	CG	LEU A		29.029	26.208	61.444	1.00 36.96
	ATOM	3181	CD1	LEU A	404	30.454	26.717	61.353	1.00 37.13
	ATOM	3182	CD2	LEU A	404	28.083	27.362	61.163	1.00 39.27
	MOTA	3183	N	GLY A	405	27.670	21.921	59.826	1.00 22.02
15	MOTA	3184	CA	GLY A		27.167	20.908	58.928	1.00 22.77
	ATOM	3185	C	GLY A		25.698	20.676	59.206	1.00 31.85
	,								
	MOTA	3186	0	GLY A		24.885	20.438	58.297	1.00 33.01
42 M.	MOTA	3187	N	PHE A		25.364	20.747	60.493	1.00 26.28
£1	MOTA	3188	CA	PHE A	406	23.992	20.565	60.863	1.00 25.27
20	ATOM	3189	С	PHE A	406	23.188	21.757	60.365	1.00 34.80
	ATOM	3190	0	PHE A		22.195	21.629	59.638	1.00 36.22
	ATOM	3191	СВ	PHE A		23.798			
4-4							20.268	62.351	1.00 24.52
IFA HER	ATOM	3192	CG	PHE A		22.388	20.525	62.798	1.00 24.82
3 FP (ATOM	3193	CD1	PHE A	406	21.328	19.734	62.353	1.00 28.50
25	ATOM	3194	CD2	PHE A	406	22.107	21.579	63.669	1.00 30.12
UT 25	ATOM	3195	CE1	PHE A	406	20.025	19.977	62.793	1.00 31.40
les.	ATOM	3196	CE2	PHE A	406	20.810	21.862	64.105	1.00 32.57
#	ATOM	3197	CZ	PHE A		19.771	21.037	63.669	
									1.00 31.88
h 20	ATOM	3198	N	LEU A		23.661	22.934	60.708	1.00 32.11
n. 30	ATOM	3199	CA	LEU A		22.972	24.132	60.269	1.00 33.11
7.	ATOM	3200	C	LEU A	407	22.706	24.204	58.767	1.00 34.74
(late	ATOM	3201	0	LEU A	407	21.635	24.615	58.341	1.00 35.21
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	MOTA	3202	СВ	LEU A	407	23.589	25.420	60.840	1.00 35.36
1945) Lauri	ATOM	3203	CG	LEU A		22.597	26,577	60.855	1.00 41.79
35	ATOM	3204	CD1	LEU A					
F 33						23.048	27.626	61.833	1.00 40.45
	ATOM	3205		LEU A		22.513	27.197	59.461	1.00 49.57
	MOTA	3206	N	LYS A		23.667	23.804	57.948	1.00 34.92
	MOTA	3207	CA	LYS Å	408	23.476	23.826	56.490	1.00 36.29
	ATOM	3208	С	LYS A	408	22.378	22.876	56.037	1.00 38.15
40	ATOM	3209	0	LYS A		21.568	23.191	55.160	1.00 35.09
	ATOM	3210	СВ	LYS A		24.747	23.517	55.707	1.00 40.54
	ATOM	3211	CG	LYS A			23.873		
						24.633		54.214	1.00 43.41
	ATOM	3212	CD	LYS A		25.950	23.796	53.422	1.00 49.26
	ATOM	3213	CE	LYS A		26.808	25.059	53.459	1.00 61.45
45	MOTA	3214	NZ	LYS A	408	28.014	24.994	52.606	1.00 73.78
	ATOM	3215	N	ALA A	409	22.352	21.690	56.655	1.00 35.34
	ATOM	3216	CA	ALA A	409	21.333	20.698	56.298	1.00 36.14
	ATOM	3217	С	ALA A		19.927	21.041	56.814	1.00 38.45
	ATOM	3218	ŏ	ALA A		18.913	20.821	56.134	1.00 37.39
50									
20	ATOM	3219	CB	ALA A		21.762	19.273	56,626	1.00 36.66
	ATOM	3220	N	TYR A		19.902	21.597	58.030	1.00 33.14
	MOTA	3221	CA	TYR A		18.693	22.059	58.682	1.00 29.65
	MOTA	3222	С	TYR A	410	18.028	23.051	57.730	1.00 35.55
	MOTA	3223	0	TYR A	410	16.855	22.976	57.399	1.00 37.26
55	MOTA	3224	СВ	TYR A		19.117	22.762	59.970	1.00 24.67
	MOTA	3225	CG	TYR A		18.069	23.643	60.541	
									1.00 26.95
	ATOM	3226		TYR A		16.861	23.112	60.990	1.00 28.10
	ATOM	3227		TYR A		18.288	25.015	60.663	1.00 29.66
	ATOM	3228		TYR A		15.883	23.924	61.571	1.00 26.98
60	ATOM	3229	CE2	TYR A	410	17.316	25.839	61.230	1.00 31.84
	ATOM	3230	CZ	TYR A		16.112	25.294	61.685	1.00 37.49
	ATOM	3231	ОН	TYR A		15.156	26.110	62.241	1.00 33.48
	ATOM	3232	N	VAL A		18.848	23.961	57.262	1.00 33.46
	ATOM	3233	CA	VAL A		18.457			
	ALON	2233	-CA	AUTH W	377	10.42/	24.984	56.341	1.00 29.23

	ATOM	3234	С	VAL A	411	18.013	24.469	54.992	1 00 04 00
	ATOM	3235							1.00 34.00
			0	VAL A		17.060	24.982	54.401	1.00 30.00
	ATOM	3236	CB	VAL A	411	19.617	25.922	56.139	1.00 32.22
	MOTA	3237	CG1	VAL A		19.331	26.821	54.950	
5.	ATOM	3238		VAL A					1.00 29.86
J						19.850	26.708	57.431	1.00 31.69
	ATOM	3239	N	GLU A	412	18.730	23.479	54.488	1.00 33.14
	ATOM	3240	CA	GLU A	412	18.402	22.900	_	
	ATOM	3241						53.217	1.00 31.91
			С	GLU A		17.068	22.163	53.355	1.00 30.32
	MOTA	3242	0	GLU A	412	16.182	22.225	52.531	1.00 31.89
10	ATOM	3243	CB	GLU A		19.502	21.883	52.932	
		3244							1.00 36.48
	ATOM		CG	GLU A		20.443	22.174	51.737	1.00 67.01
	MOTA	3245	CD	GLU A	412	21.872	21.699	51.962	1.00100.00
	ATOM	3246	OE1	GLU A	412	22.193	20.782		
	ATOM	3247		GLU A				52.716	1.00100.00
15						22.750	22.396	51.277	1.00 94.73
15	ATOM	3248	N	LYS A	413	16.922	21.444	54.444	1.00 22.18
	ATOM	3249	CA	LYS A	413	15.729	20.692	54.714	
	ATOM	3250	С	LYS A					1.00 17.91
						14.463	21.486	54.855	1.00 23.75
	ATOM	3251	0	LYS A	413	13.417	20.978	54.503	1.00 25.92
	ATOM	3252	CB	LYS A	413	15.890	19.911	55.988	
20	ATOM	3253	CG						1.00 15.65
20				LYS A		14.554	19.422	56.503	1.00 38.69
	MOTA	3254	CD	LYS A	413	14.150	18.089	55.903	1.00 58.11
	ATOM	3255	CE	LYS A		13.634	17.099		
	ATOM	3256						56.937	1.00 64.98
			NZ	LYS A		13.457	15.751	56.381	1.00 73.89
~ =	MOTA	3257	N	PHE A	414	14.530	22.688	55.424	1.00 25.40
25	MOTA	3258	CA	PHE A	414	13.316	23.479	55.640	
	ATOM	3259	С	PHE A					1.00 27.80
						13.151	24.748	54.821	1.00 35.82
	ATOM	3260	0	PHE A	414	12.276	25.557	55.122	1.00 35.17
	MOTA	3261	CB	PHE A	414	13.063	23.791	57.118	
	ATOM	3262	CG	PHE A	A 1 A	12.936			1.00 30.46
30	ATOM			- 111D A	373		22.553	57.964	1.00 33.88
30		3263	CDI	PHE A	414	11.746	21.826	57.996	1.00 35.94
	ATOM	3264	CD2	PHE A	414	14.005	22.110	58.742	1.00 37.75
	ATOM	3265	CE1	PHE A	414	11.629	20.664	58.761	
	ATOM	3266		PHE A					1.00 37.77
						13.888	20.962	59.526	1.00 42.23
25	ATOM	- 3267	CZ	PHE A		12.698	20.231	59.542	1.00 39.10
35	ATOM	3268	N	SER A	415	13.970	24.933	53.795	1.00 36.12
	MOTA	3269	CA	SER A		13.858	26.115		
	ATOM	3270	C					52.945	1.00 36.36
				SER A		12.412	26.295	52.510	1.00 38.99
	ATOM	3271	0	SER A	415	11.730	25.315	52.243	1.00 41.04
	ATOM	3272	CB	SER A	415	14.773	26.008	51.736	
40	ATOM	3273	OG						1.00 37.43
••				SER A		16.036	26.566	52.046	1.00 46.73
	ATOM	3274	N	TYR A	416	11.928	27.537	52.475	1.00 33.40
	MOTA	3275	CA	TYR A	416	10.541	27.832	52.072	
	ATOM	3276	С	TYR A					1.00 30.88
						9.453	27.183	52.947	1.00 33.62
4.5	ATOM	3277	0	TYR A	416	8.295	27.095	52.546	1.00 33.44
45	ATOM	3278	CB	TYR A	416	10.292	27.479	50.584	1.00 28.42
	ATOM	3279	CG	TYR A					
	ATOM	3280					27.782	49.723	1.00 24.76
				TYR A		11.791	29.087	49.338	1.00 26.55
	ATOM	3281	CD2	TYR A	416	12.375	26.778	49.335	1.00 21.68
	ATOM	3282	CE1	TYR A	416		29.384		
50	ATOM	3283		TYR A				48.570	1.00 25.16
-							27.052	48.572	1.00 20.15
	ATOM	3284	CZ	TYR A	416	13.780	28.360	48.189	1.00 30.62
	ATOM	3285	OH	TYR A	416		28.616	47.399	
	ATOM	3286		LYS A					1.00 35.15
							26.713	54.122	1.00 27.67
EF	ATOM	3287		LYS A		8.889	26.065	55.008	1.00 28.02
55	ATOM	3288	С	LYS A	417	8.733	26.830	56.317	
	ATOM	3289		LYS A					1.00 31.36
							27.6 7 1	56.682	1.00 33.15
	ATOM	3290		LYS A		9.335	24.615	55.252	1.00 33.86
	ATOM	3291	CG	LYS A	417		23.792	56.201	
	ATOM	3292		LYS A					1.00 86.28
60							22.275	56.232	1.00100.00
00	ATOM	3293		LYS A		7.924	21.471	57.265	1.00 72.28
	MOTA	3294	NZ	LYS A	417		20.033	57.323	1.00 41.88
	ATOM	3295		SER A		_		57.023	1.00 41.88
							26.557	57.033	1.00 28.88
	ATOM	3296		SER A		7.455	27.195	58.335	1.00 30.04
	ATOM	3297	C	SER A	418		26.064	59.332	1.00 34.09
						·		35.002	2.00 34.09

		ATOM	3298	0	SER A	418	6.	614	25.145	59.193	1.00 31.54
		ATOM	3299	CB	SER A			261	28.126	58.410	1.00 31.46
		ATOM	3300	OG	SER A			417	29.106	57.399	1.00 35.01
		ATOM	3301	N	ILE A			356	26.077	60.281	1.00 28.50
	5		3302	CA	ILE A			446			
	9	ATOM							24.971	61.205	1.00 23.86
		ATOM	3303	C	ILE A			272	25.342	62.641	1.00 25.06
		MOTA	3304	0	ILE A			122	26.500	63.002	1.00 21.64
		MOTA	3305	CB	ILE A			803	24.314	61.026	1.00 25.02
	1 0	MOTA	3306	CG1	ILE A		10.		25.325	61.399	1.00 23.63
	10	MOTA	3307		ILE A		10.	051	23.937	59.565	1.00 23.22
		ATOM	3308	CD1	ILE A	419	12.	236	24.688	61.253	1.00 23.48
		MOTA	3309	N	THR A	420	8.	321	24.302	63.455	1.00 24.71
		ATOM	3310	CA	THR A	420	8.	201	24.417	64.895	1.00 24.36
		ATOM	3311	С	THR A	420		416	23.795	65.538	1.00 28.90
	15	ATOM	3312	0	THR A	420	10.	190	23.112	64.863	1.00 23.38
		ATOM	3313	CB	THR A			979	23.691	65.448	1.00 24.92
		MOTA	3314		THR A			190	22.313	65.291	1.00 26.43
		MOTA	3315		THR A			728	24.082	64.694	1.00 20.43
and the		ATOM	3316	N	THR A			542	24.051	66.855	
PR	20	ATOM	3317	CA	THR A		10.				1.00 29.30
J)	20	ATOM	3318	C	THR A		10.		23.549	67.709	1.00 27.78
									22.035	67.585	1.00 30.99
L4 .		ATOM	3319	0	THR A		11.		21.594	67.489	1.00 33.28
		ATOM	3320	CB	THR A		10.		23.969	69.166	1.00 21.94
2 m/s 15 m/s	25	ATOM	3321		THR A		10.		25.369	69.263	1.00 24.52
(1) (1) (1) (1) (1) (1) (1) (1) (1) (1)	25	MOTA	3322	CG2	THR A		11.	399	23.221	70.045	1.00 20.12
The state of the s		MOTA	3323	N	ASP A	422	9.	721	21.272	67.575	1.00 21.94
#=#o		ATOM	3324	CA	ASP A	422	9.	706	19.823	67.430	1.00 21.08
		ATOM	3325	С	ASP A	422	10.	323	19.401	66.104	1.00 31.16
#		ATOM	3326	0	ASP A	422	11.	110	18.427	66.027	1.00 31.95
100 to	30	ATOM	3327	CB	ASP A	422	8.	276	19.278	67.561	1.00 19.49
#F (1)		ATOM	3328	CG	ASP A			236	17.802	67.298	1.00 31.85
n.		ATOM	3329	OD1	ASP A			130	17.040	67.654	1.00 29.73
		ATOM	3330		ASP A			197	17.415	66.598	1.00 56.60
Seattle.		ATOM	3331	N	ASP A			957	20.146	65.049	1.00 26.75
	35	ATOM	3332	CA	ASP A			505	19.876	63.729	1.00 26.01
∥a£.	-	ATOM	3333	c	ASP A			027	19.957	63.830	
		MOTA	3334	Õ	ASP A			753			1.00 40.09
		ATOM	3335	CB	ASP A			000	19.020	63.500	1.00 47.09
		ATOM	3336	CG	ASP A				20.833	62.631	1.00 24.86
	40		3337					538	20.722	62.343	1.00 39.90
	40	ATOM			ASP A			968	19.649	62.299	1.00 45.03
		ATOM	3338		ASP A			943	21.887	62.113	1.00 40.43
		ATOM	3339	N	TRP A			493	21.099	64.320	1.00 31.92
		ATOM	3340	CA	TRP A			903	21.372	64.495	1.00 29.69
	4.5	ATOM	3341	С	TRP A			611	20.271	65.282	1.00 33.81
	45	MOTA	3342	0	TRP A			537	19.616	64.824	1.00 35.87
		MOTA	3343	CB	TRP A			056	22.711	65.239	1.00 26.11
		MOTA	3344	CG	TRP A			431	22.869	65.786	1.00 27.05
		ATOM	3345		TRP A			518	23.302	65.101	1.00 29.65
		ATOM.	3346		TRP A		15.	885	22.587	67.119	1.00 26.62
	50	ATOM	3347		TRP A		17.	612	23.321	65.922	1.00 27.83
		ATOM	3348	CE2	TRP A	424	17.	257	22.891	67.163	1.00 28.62
		ATOM	3349	CE3	TRP A	424	15.	260	22.138	68.269	1.00 29.69
		ATOM	3350	CZ2	TRP A	424		010	22.758	68.319	1.00 29.28
		MOTA	3351		TRP A			000	21.993	69.429	1.00 33.50
	55	ATOM	3352		TRP A			362	22.317	69.459	1.00 33.93
		ATOM	3353	N	LYS A			156	20.090	66.497	1.00 28.75
		ATOM	3354	CA	LYS A			723	19.105	67.373	1.00 29.43
		ATOM	3355	C	LYS A			697	17.691	66.808	
		ATOM	3356	Õ	LYS A			627			1.00 29.49
	60	ATOM	3357	СВ	LYS A				16.928	67.030	1.00 27.65
	-	ATOM	3358	CG				078	19.171	68.744	1.00 29.70
		ATOM	3359		LYS A			860	18.414	69.787	1.00 28.11
				CD	LYS A			161	18.409	71.132	1.00 23.57
		ATOM	3360	CE	LYS A			300	17.063	71.815	1.00 36.16
		MOTA	3361	NZ	LYS A	425	13.	042	16.302	71.768	1.00 58.08

	ATOM	3362	N	ASP A 4	126	13.606	17.361	66.107	1.00 19.05
	ATOM	3363	CA	ASP A 4					
						13.417	16.070	65.516	1.00 18.43
	ATOM	3364	С	ASP A 4		14.453	15.879	64.387	1.00 28.33
_	ATOM	3365	0	ASP A 4		15.070	14.832	64.232	1.00 31.25
5	ATOM	3366	CB	ASP A 4	26	11.920	15.840	65.098	1.00 19.79
	MOTA	3367	CG	ASP A 4	26	10.998	15.575	66.274	1.00 25.54
	ATOM	3368		ASP A 4		11.341	15.466	67.409	1.00 29.73
		3369							
	ATOM			ASP A 4		9.804	15.611	65.938	1.00 20.67
10	ATOM	3370	N	PHE A 4		14.674	16.926	63.612	1.00 25.09
10	ATOM	3371	CA	PHE A 4	127	15.654	16.899	62.540	1.00 25.81
	ATOM	3372	С	PHE A 4	27	17.066	16.718	63.159	1.00 34.01
	ATOM	3373	0	PHE A 4		17.843	15.851	62.773	1.00 36.25
	ATOM	3374	СВ	PHE A 4					
						15.589	18.197	61.704	1.00 26.35
15	ATOM	3375	CG	PHE A 4		16.698	18.202	60.702	1.00 27.40
15	ATOM	3376		PHE A 4		16.714	17.247	59.686	1.00 29.97
	ATOM	3377	CD2	PHE A 4	127	17.773	19.084	60.805	1.00 28.71
	ATOM	3378	CE1	PHE A 4	127	17.730	17.194	58.733	1.00 27.72
	ATOM	3379				18.806	19.046	59.867	
	ATOM	3380	CZ	PHE A 4					1.00 30.37
20						18.780	18.104	58.837	1.00 26.34
20	MOTA	3381	N	LEU A 4		17.369	17.544	64.160	1.00 28.94
	ATOM	3382	CA	LEU A 4	128	18.622	17.496	64.924	1.00 27.74
	ATOM	3383	С	LEU A 4	128	18.989	16.047	65.303	1.00 32.08
	ATOM	3384	0	LEU A 4		20.145	15.647	65.209	1.00 36.38
	ATOM	3385	СВ	LEU A 4					
25						18.510	18.362	66.223	1.00 24.68
23	ATOM	3386	CG	LEU A 4		19.778	18.377	67.079	1.00 24.30
	ATOM	3387	CD1		128	20.855	19.278	66.467	1.00 23.00
	ATOM	3388	CD2	LEU A 4	128	19.446	18.856	68.481	1.00 16.41
	ATOM	3389	N	TYR A 4	129	17.991	15.271	65.735	1.00 23.71
	ATOM	3390	CA	TYR A 4		18.148			
30							13.896	66.144	1.00 23.18
50	ATOM	3391	C	TYR A 4		18.311	12.967	64.976	1.00 26.62
	ATOM	3392	0	TYR A 4		18.911	11.910	65.076	1.00 28.43
	ATOM	3393	CB	TYR A 4	129	16.921	13.453	66.914	1.00 25.59
	ATOM	3394	CG	TYR A 4	129	17.069	13.526	68.414	1.00 29.53
	ATOM	3395	CD1	TYR A 4	129	16.823	14.714	69.114	1.00 31.11
35	ATOM	3396		TYR A 4		17.361	12.383		
	ATOM	3397						69.156	1.00 32.70
			CE1	-		16.916	14.769	70.510	1.00 32.23
	MOTA	3398	CE2	TYR A 4		17.485	12.420	70.551	1.00 35.30
	ATOM	3399	CZ	TYR À 4	129	17.251	13.623	71.231	1.00 41.02
	MOTA	3400	OH	TYR A 4	129	17.339	13.679	72.609	1.00 30.02
40	ATOM	3401	N	SER A 4	130	17.748	13.342	63.854	1.00 21.68
	ATOM	3402	CA	SER A 4		17.914	12.469	62.730	1.00 23.42
	ATOM	3403	C	SER A 4		19.264			
	ATOM	3404	Ö				12.722	62.050	1.00 32.87
				SER A 4		19.879	11.819	61.467	1.00 35.11
4.5	ATOM	3405	CB	SER A 4		16.756	12.541	61.773	1.00 28.79
45	ATOM	3406	OG	SER A 4	130	17.089	13.475	60.777	1.00 49.56
	MOTA	3407	N	TYR A 4	131	19.748	13.955	62.132	1.00 27.18
	ATOM	3408	CA	TYR A 4		21.017	14.296	61.537	1.00 27.14
	ATOM	3409	C	TYR A 4					
						22.152	13.702	62.316	1.00 32.52
50	ATOM	3410	0	TYR A 4		23.155	13.242	61.771	1.00 33.64
50	ATOM	3411	CB	TYR A 4		21.216	15.818	61.385	1.00 31.07
	ATOM	3412	CG	TYR A 4	131	22.566	16.265	60.812	1.00 35.63
	ATOM	3413	CD1	TYR A 4	131	23.663	16.492	61.650	1.00 36.88
	ATOM	3414		TYR A 4		22.735	16.496	59.444	1.00 36.92
	ATOM	3415		TYR A 4					
55						24.894	16.924	61.157	1.00 33.78
55	MOTA	3416				23.964	16.916	58.924	1.00 37.86
	ATOM	3417	CZ	TYR A 4	131	25.038	17.143	59.786	1.00 46.01
	ATOM	3418	OH	TYR A 4	131	26.247	17.573	59.294	1.00 51.28
	ATOM	3419	N	PHE A 4		21.964	13.728	63.606	1.00 29.66
	ATOM	3420	CA	PHE A 4		22.939	13.720		
60	ATOM	3421	C					64.526	1.00 29.12
				PHE A 4		22.522	11.865	65.007	1.00 42.64
	ATOM	3422	0	PHE A 4		22.499	11.593	66.197	1.00 46.77
	MOTA	3423	СВ	PHE A 4		23.063	14.157	65.719	1.00 30.24
	MOTA	3424	CG	PHE A 4	132	23.962	15.327	65.401	1.00 33.03
	MOTA	3425	CD1	PHE A 4		25.336	15.113	65.277	1.00 37.22
						· · ·			

	ATOM	3426	CD2	PHE A	432		23.470	16,624	65.232	1.00 30.70
	ATOM	3427		PHE A			26.223	16.153	64.999	1.00 34.27
	ATOM	3428	CE2	PHE A	432		24.349	17.667	64.938	1.00 31.71
	ATOM	3429	CZ	PHE A	432		25.722	17.438	64.823	1.00 27.82
5	ATOM	3430	N	LYS A	433		22.174	11.029	64.063	1.00 42.50
	ATOM	3431	CA	LYS A			21.669	9.670	64.270	1.00 40.87
	ATOM	3432	С	LYS A	433		22.718	8.751	64.908	1.00 46.17
	ATOM	3433	0	LYS A			22.405	7.734	65.513	1.00 48.48
	ATOM	3434	CB	LYS A			21.245	9.106	62.917	1.00 39.25
10	ATOM	3435	CG	LYS A			19.988	8.241	63.017	1.00 84.17
	ATOM	3436	CD	LYS A	433		18.925	8.660	62.000	1.00100.00
	ATOM	3437	CE	LYS A			17.523	8.172	62.384	1.00100.00
	MOTA	3438	NZ	LYS A			16.525	9.119	61.884	1.00100.00
	ATOM	3439	N	ASP A	434		24.002	9.112	64.697	1.00 45.20
15	ATOM	3440	CA	ASP A	434		25.083	8.349	65.321	1.00 47.80
	MOTA	3441	С	ASP A			25.201	8.684	66.802	1.00 50.78
	ATOM	3442	0	ASP A	434		25.474	7.845	67.653	1.00 55.76
	ATOM	3443	CB	ASP A	434		26.405	8.567	64.562	1.00 53.91
	ATOM	3444	CG	ASP A	434		26.123	8.474	63.069	1.00 93.32
20	ATOM	3445	OD1	ASP A	434		25.744	7.573	62.325	1.00 96.22
43	ATOM	3446		ASP A			26.119	9.664	62.753	1.00100.00
jak.	ATOM	3447	N	LYS A	435		25.015	9.978	67.085	1.00 38.82
Barrier Barrier	ATOM	3448	CA	LYS A	435		24.974	10.404	68.468	1.00 34.57
अर्थु मार् रक्ष	ATOM	3449	С	LYS A			23.549	10.749	68.881	1.00 39.87
25	ATOM	3450	0	LYS A	435		23.070	11.840	68.693	1.00 40.34
u"	ATOM	3451	CB	LYS A	435		25.864	11.631	68.615	1.00 34.69
\$= 5 .	ATOM	3452	CG	LYS A	435		27.064	11.595	67.679	1.00 40.86
.	ATOM	3453	CD	LYS A	435		27.703	12.975	67.532	1.00 51.04
⁻ 20	ATOM	3454	CE	LYS A	435	-	29.242	12.904	67.557	1.00 24.08
30	ATOM	3455	NZ	LYS A	435		29.822	13.990	66.760	1.00 45.26
14 st	ATOM	3456	N	VAL A	436		22.843	9.728	69.414	1.00 38.07
77 3 1 46 1 46	MOTA	3457	CA	VAL A	436		21.601	10.036	70.111	1.00 36.86
44	MOTA	3458	С	VAL A	436		21.846	10.129	71.608	1.00 44.88
	MOTA	3459	0	VAL A	436		21.289	10.948	72.300	1.00 46.42
} ₄₄35	MOTA	3460	CB	VAL A	436		20.567	8.923	69.816	1.00 37.37
	MOTA	3461	CG1	VAL A	436		19.944	9.143	68.446	1.00 36.24
	ATOM	3462	CG2	VAL A	436		21.227	7.556	69.854	1.00 36.80
	ATOM	3463	N	ASP A			22.718	9.232	72.099	1.00 43.61
•	ATOM	3464	CA	ASP A			23.044	9.222	73.522	1.00 41.43
40	ATOM	3465	С	ASP A			23.657	10.546	73.958	1.00 45.71
	ATOM	3466	0	ASP A			23.554	10.956	75.107	1.00 49.89
	MOTA	3467	CB	ASP A			24.022	8.082	73.776	1.00 43.84
	ATOM	3468	CG	ASP A			23.281	6.752	73.691	1.00 72.47
4.5	ATOM	3469		ASP A			22.062	6.769	73.823	1.00 74.64
45	ATOM	3470		ASP A			23.933	5.730	73.481	1.00 86.09
	ATOM	3471	N	VAL A			24.333	11.324	73.122	1.00 40.21
	ATOM	3472	CA	VAL A			24.807		73.577	1.00 40.97
	ATOM	3473	С	VAL A			23.621	13.582	73.668	1.00 41.86
50	ATOM	3474	0	VAL A			23.368	14.276	74.657	1.00 39.95
50	ATOM	3475	CB	VAL A			25.875	13.165	72.615	1.00 47.47
	MOTA	3476		VAL A			26.438	14.523	73.051	1.00 47.51
	ATOM	3477		VAL A			26.996	12.149	72.440	1.00 47.51
	ATOM	3478	N	LEU A			22.876	13.595	72.585	1.00 37.91
55	MOTA	3479	CA	LEU A			21.729	14.442	72.507	1.00 36.21
33	ATOM	3480	C	LEU A			20.850	14.190	73.695	1.00 40.03
	ATOM	3481	0	LEU A			20.214	15.064	74.255	1.00 42.22
	ATOM	3482	CB	LEU A			20.949	14.180	71.210	1.00 33.84
	ATOM	3483	CG	LEU A			21.552	14.939	70.039	1.00 32.80
<i>د</i> ۸	ATOM	3484		LEU A			20.813	14.538	68.775	1.00 34.08
60	ATOM	3485		LEU A			21.435	16.434	70.258	1.00 23.80
	ATOM	3486	N	ASN A			20.810	12.953	74.076	1.00 34.03
	ATOM	3487	CA	ASN A			19.971	12.603	75.187	1.00 34.00
	ATOM	3488	C	ASN A			20.494	13.093	76.532	1.00 40.95
	ATOM	3489	0	ASN A	440		19.816	12.995	77.544	1.00 42.09

	ATOM	3490	CB	ASN A	440	19.681	11.095	75.178	7 00 24 00
	ATOM	3491	CG	ASN A					1.00 24.89
						18.790	10.635	74.028	1.00 46.52
	ATOM	3492	OD.	L ASN A	440	19.005	9.537	73.480	1.00 58.82
	ATOM	3493	ND2	ASN A	440	17.769	11.440	73.680	1.00 31.11
5	ATOM	3494	N	GLN A		21.707			
							13.623	76.531	1.00 36.98
	ATOM	3495	CA	GLN A		22.339	14.095	77.744	1.00 35.47
	ATOM	3496	С	GLN A	441	21.879	15.478	78.067	1.00 36.00
	ATOM	3497	0	GLN A				70.007	
						22.137	16.029	79.142	1.00 34.96
	MOTA	3498	CB	GLN A	441	23.878	14.109	77.581	1.00 38.10
10	ATOM	3499	CG	GLN A	441	24.504	12.692	77.422	
	ATOM	3500	CD	GLN A					1.00 52.06
						25.954	12.730	76.955	1.00 81.69
	ATOM	3501	OE1	GLN A	441	26.476	13.796	76.609	1.00 74.46
	ATOM	3502	NE2	GLN A	441	26.616	11.574		
	ATOM	3503	N					76.972	1.00 91.09
15				VAL A		21.197	16.067	77.112	1.00 31.86
15	ATOM	3504	CA	VAL A	442	20.753	17.411	77.384	1.00 32.78
	MOTA	3505	С	VAL A	442	19.354	17.468		
	ATOM	3506	ō					77.970	1.00 38.24
				VAL A		18.468	16.700	77.588	1.00 42.83
	ATOM	3507	CB	VAL A	442	20.845	18.277	76.159	1.00 34.84
	MOTA	3508	CG1	VAL A	442	21.430	17.435		
20								75.020	1.00 34.65
20	MOTA	3509		VAL A		19.441	18.705	75.811	1.00 33.21
	ATOM	3510	N	ASP A	443	19.172	18.388	78.908	1.00 25.60
	ATOM	3511	CA	ASP A		17.931			
	ATOM						18.634	79.616	1.00 24.57
		3512	С	ASP A		16.996	19.533	78.791	1.00 32.14
	ATOM	3513	0	ASP A	443	16.744	20.732	79.073	1.00 34.77
25	ATOM	3514	СВ	ASP A		18.332	19.272		
	ATOM							80.957	1.00 27.11
		3515	CG	ASP A		17.216	19.413	81.901	1.00 39.99
	ATOM	3516	OD1	ASP A	443	16.063	19.234	81.573	1.00 44.78
	ATOM	3517	OD2	ASP A	443	17.631	19.753		
	ATOM	3518						83.094	1.00 56.66
20			N	TRP A		16.525	18.914	77.722	1.00 28.30
30	ATOM	3519	CA	TRP A	444	15.614	19.507	76.757	1.00 26.27
	ATOM	3520	С	TRP A	444	14.460	20.296		
	ATOM	3521						77.416	1.00 31.52
			0	TRP A		14.102	21.409	76.988	1.00 34.63
	ATOM	3522	CB	TRP A		15.067	18.398	75.799	1.00 21.47
	ATOM	3523	CG	TRP A	444	16.095	17.951	74.806	
35	ATOM	3524	CD1						1.00 22.03
						16.675	16.718	74.736	1.00 25.16
	ATOM	3525	CD2	TRP A	444	16.733	18.738	73.776	1.00 20.36
	MOTA	3526	NE1	TRP A	444	17.623	16.677	73.738	
	ATOM	3527	CE2						1.00 23.97
						17.688	17.906	73.138	1.00 24.71
40	ATOM	3528	CE3			16.596	20.045	73.342	1.00 20.86
40	ATOM	3529	CZ2	TRP A	444	18.448	18.345	72.060	1.00 24.51
	MOTA	3530	CZ3			17.353			
	ATOM						20.471	72.264	1.00 22.88
		3531	CH2			18.281	19.643	71.643	1.00 23.48
	MOTA	3532	N	ASN A	445	13.855	19.711	78.457	1.00 24.92
	ATOM	3533	CA	ASN A		12.723	20.326		
45	ATOM	3534						79.113	1.00 26.30
			С	ASN A		13.040	21.677	79.729	1.00 30.17
	MOTA	3535	0	ASN A	445	12.291	22.660	79.547	1.00 31.86
	ATOM	3536	CB	ASN A	445	11.987	19.382	80.094	
	ATOM	3537	CG	ASN A					1.00 40.83
				AUN A	443	10.946	20.033	81.020	1.00 87.07
FΛ	ATOM	3538	ODI	ASN A	445	11.271	20.635	82.065	1.00 86.38
50	ATOM	3539	ND2	ASN A	445	9.670	19.848	80.688	1.00 71.65
•	ATOM	3540	N	ALA A		14.147			
							21.687	80.436	1.00 22.70
	ATOM	3541	CA	ALA A		14.583	22.886	81.073	1.00 24.45
	ATOM	3542	С	ALA A	446	14.886	23.896	79.990	
	ATOM	3543	0	ALA A		14.324			1.00 30.52
55							25.001	79.936	1.00 33.92
55	ATOM	3544	CB	ALA A		15.814	22.543	81.900	1.00 25.68
	ATOM	3545	N	TRP A	447	15.776	23.494	79.102	1.00 25.24
	ATOM	3546	CA	TRP A					
						16.162	24.384	78.034	1.00 26.83
	ATOM	3547	С	TRP A		14.989	24.912	77.223	1.00 31.32
	ATOM	3548	0	TRP A	447	14.971	26.089	76.875	1.00 30.48
60	ATOM	3549	CB	TRP A		17.166			
	ATOM						23.725	77.062	1.00 25.78
		3550	CG	TRP A		18.625	23.815	77.421	1.00 26.60
	ATOM	3551	CD1			19.343	22.840	78.046	1.00 28.89
	MOTA	3552	CD2	TRP A		19.554	24.896	77.165	1 00 00 10
	ATOM	3553		TRP A					1.00 26.16
	111 011	2222	1151	TUL H	44/	20.654	23.217	78.197	1.00 27.23

	ATOM	3554	CE2	TRP A 447	20.822	24.476	77.660	1.00 29.00
	ATOM	3555				26.162	76.607	
				TRP A 447	19.435			1.00 27.56
	ATOM	3556		TRP A 447	21.954	25.290	77.583	1.00 27.95
_	ATOM	3557		TRP A 447	20.554	26.966	76.538	1.00 29.93
5	MOTA	3558		TRP A 447	21.792	26.539	77.035	1.00 30.16
	MOTA	3559	N	LEU A 448	14.029	24.034	76.893	1.00 26.54
	MOTA	3560	CA	LEU A 448	12.896	24.421	76.052	1.00 26.92
	ATOM	3561	С	LEU A 448	11.734	25.064	76.779	1.00 36.15
10	MOTA	3562	0	LEU A 448	11.089	26.031	76.304	1.00 31.19
10	MOTA	3563	CB	LEU A 448	12.338	23.197	75.307	1.00 25.26
	MOTA	3564	CG	LEU A 448	13.311	22.545	74.332	1.00 28.29
	MOTA	3565		LEU A 448	12.597	21.455	73.530	1.00 30.49
	ATOM	3566		LEU A 448	13.879	23.576	73.375	1.00 21.94
	MOTA	3567	N	TYR A 449	11.472	24.455	77.924	1.00 33.14
15	MOTA	3568	CA	TYR A 449	10.373	24.835	78.747	1.00 30.64
	MOTA	3569	С	TYR A 449	10.646	25.525	80.041	1.00 34.31
	MOTA	3570	0	TYR A 449	9 .7 50	26.191	80.529	1.00 41.98
	MOTA	3571	CB	TYR A 449	9.400	23.674	78.916	1.00 29.14
	MOTA	3572	CG	TYR A 449	9.212	23.089	77.556	1.00 26.50
20	ATOM	3573	CD1	TYR A 449	8.762	23.869	76.485	1.00 24.36
	ATOM	3574	CD2	TYR A 449	9.560	21.762	77.325	1.00 28.48
	MOTA	3575	CE1	TYR A 449	8.626	23.331	75.202	1.00 17.56
	ATOM	3576	CE2	TYR A 449	9.427	21.205	76.054	1.00 29.93
	ATOM	3577	CZ	TYR A 449	8.959	21.988	74.998	1.00 33.65
25	MOTA	3578	OH	TYR A 449	8.840	21.415	73.762	1.00 39.47
	MOTA	3579	N	SER A 450	11.806	25.413	80.644	1.00 22.72
	ATOM	3580	CA	SER A 450	11.902	26.149	81.900	1.00 21.21
	MOTA	3581	С	SER A 450	12.278	27.625	81.749	1.00 23.98
	ATOM	3582	0	SER A 450	12.966	28.035	80.810	1.00 27.17
30	ATOM	3583	CB	SER A 450	12.666	25.436	83.010	1.00 24.83
	ATOM	3584	OG	SER A 450	12.540	24.046	82.871	1.00 36.29
	ATOM	3585	N	PRO A 451	11.806	28.430	82.689	1.00 19.76
	MOTA	3586	CA	PRO A 451	12.111	29.840	82.669	1.00 18.20
	ATOM	3587	С	PRO A 451	13.461	29.988	83.271	1.00 21.72
35	ATOM	3588	Ō	PRO A 451	14.022	29.015	83.742	1.00 24.34
	MOTA	3589	СВ	PRO A 451	11.185	30.485	83.695	1.00 18.85
	ATOM	3590	CG	PRO A 451	10.836	29.390	84.677	1.00 23.13
	ATOM	3591	CD	PRO A 451	11.002	28.078	83.900	1.00 19.61
	ATOM	3592	N	GLY A 452	13.959	31.212	83.307	1.00 18.97
40	ATOM	3593	CA	GLY A 452	15.241	31.444	83.922	1.00 19.09
	ATOM	3594	C	GLY A 452	16.382	31.107	83.016	1.00 26.20
	ATOM	3595	Õ	GLY A 452	16.191	30.916	81.819	1.00 27.37
	ATOM	3596	N	LEU A 453	17.557	31.057	83.650	1.00 25.48
	ATOM	3597	CA	LEU A 453	18.843	30.750	83.029	1.00 25.32
45	ATOM	3598	C	LEU A 453	18.906	29.322	82.629	1.00 26.21
	ATOM	3599	ō	LEU A 453	18.400	28.458	83.322	1.00 25.04
	ATOM	3600	CB	LEU A 453	20.042	31.119	83.938	1.00 25.46
	ATOM	3601	CG	LEU A 453	20.280	32.632	83.904	1.00 31.82
	ATOM	3602		LEU A 453	21.019	33.087	85.119	1.00 31.78
50	ATOM	3603		LEU A 453	21.046	33.056	82.651	1.00 41.50
	ATOM	3604	N	PRO A 454	19.510	29.082	81.489	1.00 22.97
	MOTA	3605	CA	PRO A 454	19.585	27.747	81.003	1.00 21.60
	ATOM	3606	C	PRO A 454	20.145	26.890	82.075	1.00 26.94
	ATOM	3607	Õ	PRO A 454	20.923	27.359	82.893	1.00 20.94
55	ATOM	3608	СВ	PRO A 454	20.489	27.780	79.768	1.00 22.34
	ATOM	3609	CG	PRO A 454	20.777	29.232	79.470	1.00 23.69
	ATOM	3610	CD	PRO A 454	20.136	30.054	80.556	1.00 23.89
	ATOM	3611	N	PRO A 455	19.721	25.648	82.067	1.00 20.82
	ATOM	3612	CA	PRO A 455	20.167	24.683	83.031	1.00 23.61
60	MOTA	3613	C	PRO A 455	21.661	24.568	82.991	1.00 24.27
00	ATOM	3614	o	PRO A 455	22.225	24.062	83.920	1.00 30.95
	ATOM	3615	CB	PRO A 455	19.631	23.320	82.592	1.00 33.47
	ATOM	3616	CG	PRO A 455	19.149	23.497	81.162	1.00 23.04
	ATOM	3617	CD	PRO A 455	19.111	25.005	80.888	1.00 33.02
	2	J		1 11 100		20.000	55.555	1.00 20.49

	MOTA	3618	N	ILE A	456	22.305	25.002	81.911	1.00 27.9
	ATOM	3619	CA	ILE A	456	23.764	24.893	81.821	1.00 27.8
	ATOM	3620	С	ILE A		24.395	26.057	81.077	1.00 34.7
_	MOTA	3621	0	ILE A		23.737	26.769	80.293	1.00 37.0
5	ATOM	3622	CB	ILE A		24.228	23.540	81.259	1.00 31.3
	ATOM	3623	CG1			25.721	23.305	81.417	1.00 29.7
	ATOM	3624		ILE A		23.865	23.369	79.788	1.00 32.9
	MOTA	3625	CD1	ILE A		26.054	21.852	81.116	1.00 23.9
10	ATOM	3626	N	LYS A		25.680	26.252	81.334	1.00 30.5
10	ATOM	3627	CA	LYS A		26.405	27.335	80.707	1.00 30.2
	ATOM	3628	С	LYS A		27.515	26.808	79.835	1.00 32.1
	MOTA	3629	0	LYS A		28.328	26.037	80.273	1.00 33.0
	ATOM	3630	CB	LYS A		26.953	28.264	81.749	1.00 32.3
1.5	ATOM	3631	CG	LYS A		27.818	29.327	81.121	1.00 34.64
15	ATOM	3632	CD	LYS A		28.288	30.306	82.166	1.00 13.43
	ATOM	3633	CE	LYS A		28.803	31.596	81.565	1.00 18.04
	ATOM	3634	NZ	LYS A		28.974	32.643	82.595	1.00 26.73
	ATOM	3635	N	PRO F		27.567	27.208	78.589	1.00 27.50
20	ATOM	3636	CA	PRO A		28.630	26.675	77.737	1.00 26.85
20	ATOM	3637	С	PRO A		29.994	27.147	78.185	1.00 26.89
 er og fikali	ATOM	3638	0	PRO A		30.128	27.876	79.167	1.00 24.86
	MOTA	3639	СВ	PRO P		28.335	27.191	76.316	1.00 29.41
	ATOM	3640	CG	PRO P		26.952	27.864	76.375	1.00 33.24
25	ATOM	3641	CD	PRO A		26.574	28.044	77.848	1.00 26.12
25	ATOM	3642	N	ASN A		31.005	26.754	77.440	1.00 22.13
	ATOM	3643	CA	ASN A		32.359	27.191	77.735	1.00 22.29
	MOTA	3644	С	ASN A		32.751	28.325	76.820	1.00 30.27
	ATOM	3645	0	ASN A		32.451	28.296	75.617	1.00 32.89
30	ATOM	3646	CB	ASN A		33.315	26.060	77.494	1.00 25.03
30	ATOM	3647	CG	ASN A		32.766	24.846	78.155	1.00 49.54
	ATOM	3648		ASN A		32.618	24.822	79.383	1.00 50.09
	ATOM	3649		ASN A		32.411	23.870	77.332	1.00 38.39
	MOTA	3650 3651	N	TYR A		33.448	29.316	77.380	1.00 25.58
35	ATOM ATOM	3652	CA	TYR A		33.851	30.493	76.625	1.00 23.89
	ATOM	3653	С 0	TYR A		35.298	30.853	76.745	1.00 34.20
	ATOM	3654	СВ	TYR A		35.849	30.862	77.839	1.00 35.27
	ATOM	3655	CG	TYR A		33.120	31.708	77.171	1.00 24.38
	ATOM	3656		TYR A	460	31.636 31.029	31.631	77.024	1.00 26.98
40	ATOM	3657		TYR A		30.838	32.011	75.829	1.00 30.69
	ATOM	3658	CE1	TYR A	460	29.644	31.168 31.952	78.064	1.00 25.70
	ATOM	3659		TYR A		29.453	31.932	75.684 77.938	1.00 28.77
	ATOM	3660	CZ	TYR A		28.863	31.496	76.741	1.00 25.24
	ATOM	3661	OH	TYR A		27.519	31.443	76.587	1.00 24.49
45	ATOM	3662		ASP A		35.893	31.227	75.616	1.00 20.58
	ATOM	3663		ASP A		37.268	31.640	75.654	1.00 30.50
	ATOM	3664		ASP A		37.319	32.941	76.464	1.00 27.51
	ATOM	3665		ASP A		36.377	33.704	76.396	1.00 26.62
	ATOM	3666		ASP A		37.821	31.784	74.218	1.00 20.02
50	ATOM	3667	CG	ASP A	461	39.137	32.466	74.260	1.00 32.53
	MOTA	3668	OD1	ASP A	461	39.262	33.672	74.334	1.00 32.56
	MOTA	3669	OD2	ASP A	461	40.130	31.628	74.306	1.00 44.34
	ATOM	3670	N	MET A	462	38.375	33.234	77.224	1.00 17.26
	MOTA	3671	CA	MET A	462	38.396	34.511	78.008	1.00 18.66
55	ATOM	3672	С	MET A	462	39.299	35.634	77.485	1.00 24.02
	ATOM	3673		MET A		39.336	36.738	78.011	1.00 24.56
	ATOM	3674		MET A		38.818	34.186	79.431	1.00 22.99
	ATOM	3675		MET A		37.808	33.209	80.025	1.00 28.98
<i>6</i> 0	ATOM	3676		MET A		36.166	33.969	79.951	1.00 33.22
60	ATOM	3677		MET A		36.420	35.300	81.153	1.00 27.89
	ATOM	3678		THR A		40.067	35.348	76.461	1.00 22.57
	ATOM	3679		THR A		41.015	36.285	75.911	1.00 22.64
	ATOM	3680		THR A		40.690	37.738	75.961	1.00 33.12
	ATOM	3681	0	THR A	463	41.372	38.493	76.640	1.00 35.27

	ATOM	3682	CB	THR A	463	41.574	35.929	74 526	1 00 00 00
	ATOM	3683	OG1			41.939	34.576	74.536	1.00 29.80
	ATOM	3684	CG2			42.797	36.793	74.509 74.224	1.00 26.74 1.00 18.79
	ATOM	3685	N	LEU A		39.700	38.141	75.177	
5	ATOM	3686	CA	LEU A		39.293	39.533		1.00 30.50
- -	ATOM	3687	c	LEU A		38.490	40.067	75.061	1.00 29.15
	ATOM	3688	Õ	LEU A		38.439		76.216	1.00 34.24
	ATOM	3689	СВ	LEU A		38.537	41.270	76.422	1.00 37.12
	ATOM	3690	CG	LEU A			39.767	73.743	1.00 29.20
10	ATOM	3691		LEU A		39.393	39.394	72.527	1.00 33.73
	ATOM	3692		LEU A		38.609 40.648	39.565	71.217	1.00 32.72
	ATOM	3693	N N	THR A			40.261	72.499	1.00 26.22
	ATOM	3694	CA	THR A		37.855	39.167	76.964	1.00 30.71
	ATOM	3695	C	THR A		37.005	39.496	78.103	1.00 28.58
15	ATOM	3696	õ	THR A		37.800	39.893	79.324	1.00 30.69
10	ATOM	3697	СВ	THR A		37.530	40.865	80.030	1.00 31.27
	ATOM	3698		THR A		36.016	38.328	78.372	1.00 35.85
	ATOM	3699		THR A		35.101	38.212	77.296	1.00 50.93
	ATOM	3700	N			35.255	38.451	79.690	1.00 26.34
20	ATOM	3701	CA	ASN A		38.802	39.111	79.568	1.00 24.40
20				ASN A		39.635	39.375	80.688	1.00 23.11
	ATOM	3702	C	ASN A		39.899	40.856	80.967	1.00 28.37
	ATOM	3703	0	ASN A		39.763	41.270	82.120	1.00 27.03
	ATOM	3704	CB	ASN A		40.921	38.543	80.629	1.00 20.30
25	ATOM	3705	CG	ASN A		40.709	37.145	81.155	1.00 32.26
23	ATOM	3706		ASN A		41.384	36.191	80.723	1.00 29.29
4	ATOM	3707		ASN A		39.775	37.015	82.111	1.00 28.19
	ATOM	3708	N	ALA A		40.306	41.666	79.967	1.00 27.97
	ATOM	3709	CA	ALA A		40.587	43.079	80.295	1.00 26.66
30	ATOM	3710	C	ALA A		39.352	43.827	80.720	1.00 31.78
30	ATOM	3711	0	ALA A		39.406	44.845	81.393	1.00 31.71
	ATOM	3712	CB	ALA A		41.365	43.837	79.256	1.00 25.99
	ATOM	3713	N	CYS A		38.217	43.277	80.336	1.00 28.06
	ATOM	3714	CA	CYS A		36.942	43.862	80.693	1.00 25.80
35	ATOM	3715	С	CYS A		36.668	43.619	82.165	1.00 26.47
33	ATOM	3716	0	CYS A		36.469	44.517	82.963	1.00 27.99
	ATOM	3717	CB	CYS A		35.882	43.376	79.696	1.00 24.56
	ATOM	3718	SG	CYS A		36.455	43.873	78.049	1.00 27.76
	ATOM	3719	N	ILE A		36.752	42.384	82.540	1.00 24.34
40	ATOM	3720	CA	ILE A		36.599	42.052	83.921	1.00 25.23
40	MOTA	3721	C	ILE A		37.560	42.800	84.876	1.00 28.13
	ATOM	3722	0	ILE A		37.175	43.220	85.950	1.00 29.54
	ATOM	3723	CB	ILE A		36.858	40.574	84.068	1.00 27.23
	ATOM	3724		ILE A		35.956	39.801	83.112	1.00 26.94
45	ATOM	3725		ILE A		36.537	40.208	85.496	1.00 25.56
43	ATOM	3726		ILE A		36.247	38.298	83.085	1.00 45.50
	ATOM	3727	N	ALA A		38.830	42.960	84.534	1.00 23.28
	ATOM	3728	CA	ALA A		39.749	43.621	85.461	1.00 22.23
	ATOM	3729	C	ALA A		39.392	45.038	85.808	1.00 30.29
50	MOTA MOTA	3730 3731	O	ALA A		39.474	45.451	86.986	1.00 32.82
50	ATOM		CB	ALA A		41.218	43.502	85.074	1.00 21.98
	ATOM	3732 3733	N CA	LEU A		39.007	45.760	84.759	1.00 23.53
	ATOM	3734		LEU A		38.643	47.173	84.834	1.00 18.39
	ATOM		C	LEU A		37.333	47.373	85.569	1.00 26.57
55	ATOM	3735 3736	O CB	LEU A		37.210	48.208	86.462	1.00 30.48
55			CB	LEU A		38.676	47.827	83.444	1.00 15.51
	MOTA	3737	CG	LEU A		38.671	49.325	83.539	1.00 24.20
	ATOM	3738		LEU A		39.754	49.795	84.513	1.00 24.86
	ATOM	3739		LEU A		38.876	49.941	82.156	1.00 26.35
60	ATOM	3740	N	SER A		36.351	46.570	85.222	1.00 25.31
UU	ATOM	3741	CA	SER A		35.080	46.674	85.901	1.00 27.56
	ATOM	3742	С	SER A		35.260	46.477	87.396	1.00 33.46
	ATOM	3743	O	SER A		34.800	47.292	88.214	1.00 32.85
	ATOM ATOM	3744	CB .	SER A		33.989	45.714	85.393	1.00 32.06
	ATOM	3745	OG	SER A	4/2	34.492	44.774	84.470	1.00 48.56

		ATOM	3746	N	GLN A	473	5	35.911	45.350	87.736	1.00	27.52
		ATOM	3747	CA	GLN A			36.170	44.971	89.108		24.10
		ATOM	3748	C	GLN A							
								36.866	46.096	89.836		25.18
	_	ATOM	3749	0	GLN A			36.534	46.458	90.969	1.00	21.62
	5	ATOM	3750	CB	GLN A			36.994	43.671	89.148	1.00	25.86
		MOTA	3751	CG	GLN A	473	3	36.128	42.402	89.118	1.00	32.72
		ATOM	3752	CD	GLN A			34.970	42.504	90.090		46.08
		ATOM	3753	OE1	GLN A			35.165				
									42.422	91.308		40.73
	10	ATOM	3754	NE2	GLN A			33.761	42.692	89.559		28.28
	10	ATOM	3755	N	ARG A	474	3	37.855	46.656	89.161	1.00	24.00
		ATOM	3756	CA	ARG A	474	3	38.562	47.765	89.779	1.00	24.46
		ATOM	3757	С	ARG A	474		37.609	48.893	90.141		29.31
		MOTA	3758	Ō	ARG A			37.620	49.447	91.242		
												33.13
	15	ATOM	3759	CB	ARG A			39.682	48.290	88.898		20.19
	15	ATOM	3760	CG	ARG A			10.866	47.352	88.831		28.48
		MOTA	3761	CD	ARG A	474	4	11.871	47.869	87.832	1.00	34.41
		MOTA	3762	NE	ARG A	474	14	12.258	49.245	88.093		40.09
		ATOM	3763	CZ	ARG A			12.927	49.938	87.185		51.25
			3764									
	20	MOTA			ARG A			13.220	49.376	86.019		24.79
	20	MOTA	3765		ARG A			13.316	51.199	87.444	1.00	20.43
,		MOTA	3766	N	TRP A			36.791	49.259	89.178	1.00	25.32
		ATOM	3767	CA	TRP A	475	3	35.862	50.332	89.400	1.00	26.77
12. 12.		ATOM	3768	С	TRP A			34.881	49.962	90.474		27.52
(a)		ATOM	3769	ō	TRP A			34.749	50.633	91.475		
n.	25											29.64
2	23	ATOM	3770	CB	TRP A			35.199	50.804	88.093		27.95
ią.		ATOM	3771	CG	TRP F			36.047	51.819	87.361	1.00	32.11
		ATOM	3772	CD1	TRP A	475	. 3	36.873	51.592	86.298	1.00	35.65
		ATOM	3773	CD2	TRP A	475		36.161	53.217	87.648		31.62
÷.		ATOM	3774	NE1				37.484	52.748	85.904		34.92
	30	MOTA	3775	CE2								
	50							37.054	53.763	86.707		36.16
8		ATOM	3776		TRP A			35.588	54.040	88.606	1.00	32.63
		ATOM	3777		TRP A			37.372	55.112	86.719	1.00	36.24
}		ATOM	3778	CZ3	TRP A	475	. 3	35.897	55.375	88.616	1.00	34.74
		ATOM	3779		TRP A			36.777	55.901	87.685		35.77
Ġ.	35	ATOM	3780	N	ILE A			34.234	48.847	90.279		26.36
		ATOM	3781	CA								
					ILE A		'	33.268	48.386	91.235		28.33
		MOTA	3782	C	ILE A			33.771	48.315	92.681	1.00	34.20
		ATOM	3783	0	ILE A	476	3	33.056	48.595	93.637	1.00	36.89
		ATOM	3784	CB	ILE A	476	3	32.722	47.070	90.761	1.00	32.23
	40	ATOM	3785	CG1	ILE A	476		31.993	47.308	89.443		30.49
		MOTA	3786	CG2				31.864	46.376	91.851		34.86
		ATOM	3787		ILE A							
								31.595	46.005	88.756		33.04
		ATOM	3788	N	THR A			35.010	47.934	92.860	1.00	27.27
		ATOM	3789	CA	THR A	477	3	35.558	47.846	94.194	1.00	24.15
	45	ATOM	3790	С	THR A	477	3	36.416	49.052	94.523	1.00	27.30
		ATOM	3791	0	THR A	477		37.120	49.065	95.519		27.36
		ATOM	3792	CB	THR A			36.402	46.578	94.257		32.13
		ATOM	3793		THR A							
								37.593	46.848	93.557		29.48
	50	ATOM	3794		THR A			35.634	45.470	93.530	1.00	16.94
	50	ATOM	3795	N	ALA A			36.371	50.097	93.695	1.00	22.33
		ATOM	3796	CA	ALA A	478	3	37.164	51.260	93.988	1.00	20.44
		ATOM	3797	С	ALA A			36.890	51.843	95.390		32.94
		ATOM	3798	0	ALA A			35.786	51.756			
										95.922		34.38
	55	ATOM	3799	CB	ALA A			36.938	52.343	92.942		19.26
	در	ATOM	3800	N	LYS A			37.931	52.469	95.970		29.65
		ATOM	3801	CA	LYS A	479	1 3	37.899	53.168	97.243	1.00	27.30
		ATOM	3802	С	LYS A	479		38.575	54.512	97.051		36.54
		MOTA	3803	0	LYS A			39.378	54.692	96.118		34.13
		ATOM	3804	СВ	LYS A			38.457				
	60								52.410	98.417		28.01
	OU,	ATOM	3805	CG	LYS A			37.696	51.116	98.631		51.38
		MOTA	3806	CD	LYS A			37.115		100.021		67.24
		ATOM	3807	CE	LYS A			35.804	50.103	99.931	1.00	87.12
		MOTA	3808	NZ	LYS A	479		35.711	48.948	100.841		85.55
		ATOM	3809	N	GLU A			38.241	55.477	97.900		36.30
		,	1.5		•							

	ATOM	3810	CA	GLU	Α	480	38.843	56.793	97.751	1.00 34.79
	ATOM	3811	C	GLU			40.261	56.707	97.220	1.00 34.79
	MOTA	3812	Ō	GLU			40.613	57.332	96.234	1.00 34.10
1.7	ATOM	3813	СВ	GLU			38.899	57.565	99.078	1.00 36.21
5	ATOM	3814	CG	GLU			37.709	58.500	99.303	1.00 63.85
,		3815	CD	GLU						
	MOTA						37.601	59.511	98.214	1.00100.00
	ATOM	3816	OE1	GLU			38.457	59.648	97.357	1.00100.00
	ATOM	3817	OE2	GLU			36.491	60.209	98.288	1.00100.00
10	ATOM	3818	N	ASP			41.080	55.946	97.904	1.00 24.69
10		3819	CA	ASP			42.451	55.860	97.519	1.00 23.87
	MOTA	3820	С	ASP	A	481	42.771	55.314	96.132	1.00 34.51
	MOTA	3821	0	ASP	Α	481	43.925	55.312	95.721	1.00 39.44
	MOTA	3822	CB	ASP	Α	481	43.262	55.155	98.611	1.00 25.29
	MOTA	3823	CG	ASP	A	481	43.072	53.668	98.575	1.00 39.58
15	MOTA	3824	OD1	ASP	Α	481	42.471	53.029	97.708	1.00 46.00
	ATOM	3825		ASP			43.698	53.107	99.567	1.00 39.59
	MOTA	3826	N	ASP			41.788	54.881	95.373	1.00 30.70
	ATOM	3827	CA	ASP			42.098	54.379	94.024	1.00 30.70
那 爾。		3828	C	ASP				55.307		
20	ATOM						41.725		92.859	1.00 34.17
		3829	O	ASP			42.158	55.150	91.717	1.00 35.45
uj	ATOM	3830	СВ	ASP			41.399	53.022	93.756	1.00 33.31
j=4 .	MOTA	3831	CG	ASP			41.686	51.970	94.779	1.00 38.90
# 2 *** *	ATOM	3832		ASP			42.810	51.514	94.992	1.00 42.45
सर्वे स्थाः	ATOM	3833	OD2	ASP			40.606	51.625	95.440	1.00 40.17
25	MOTA	3834	N	LEU	Α	483	40.863	56.246	93.146	1.00 29.93
UT.	ATOM	3835	CA	LEU	Α	483	40.352	57.159	92.160	1.00 27.80
- - -	ATOM	3836	С	LEU	Α	483	41.434	57.943	91.410	1.00 40.70
#	ATOM	3837	0	LEU	Α	483	41.386	58.102	90.180	1.00 40.76
₩_A	ATOM	3838	CB	LEU	Α	483	39.265	58.049	92.819	1.00 22.54
30) ATOM	3839	CG	LEU	Α	483	38.148	57.240	93.488	1.00 20.75
	ATOM	3840	CD1	LEU	Α	483	37.170	58.165	94.197	1.00 19.29
73	ATOM	3841	CD2	LEU	Α	483	37.389	56.467	92.414	1.00 21.46
43	ATOM		N	ASN	Α	484	42.410	58.446	92.162	1.00 36.15
a ^{r o}	MOTA		CA	ASN			43.459	59.225	91.571	1.00 34.08
35	ATOM		С			484	44.168	58.524	90.429	1.00 39.51
il and a second	ATOM	3845	0	ASN	Α	484	44.456	59.091	89.359	1.00 38.59
	ATOM		CB			484	44.495	59.602	92.618	1.00 34.26
	ATOM		CG			484	45.807	59.955	91.941	1.00100.00
	ATOM			ASN			45.878	60.940	91.171	1.00100.00
4() ATOM			ASN			46.836	59.134	92.186	1.00100.00
	ATOM		N			485	44.472	57.268	90.698	1.00 35.37
	ATOM		CA			485	45.202	56.417	89.791	1.00 32.79
	ATOM		c			485	44.522	56.140	88.484	1.00 32.26
	ATOM		0			485	45.159	55.925	87.463	1.00 32.44
4:	5 ATOM	2054	СВ			485	45.565	55.132	90.477	1.00 38.65
	ATOM		OG			485	46.040	55.437	91.777	1.00 62.66
	ATOM		N			486	43.222	56.110	88.491	1.00 27.13
	ATOM		CA			486	42.631	55.809	87.233	1.00 28.26
	ATOM		c			486	43.193	56.772	86.264	1.00 32.12
5	MOTA 0		ŏ			486	43.423	57.910	86.604	1.00 32.12
	ATOM		СВ			486	41.101	55.819	87.198	1.00 32.02
	ATOM		CG			486	40.471	54.807		
	ATOM			PHE			40.504		88.132 87.911	1.00 27.04
	ATOM			PHE				53.425		1.00 22.43
5.	,			PHE			39.805	55.293	89.253	1.00 21.40
٥.							39.896	52.538	88.804	1.00 19.69
	ATOM			PHE			39.224	54.426	90.174	1.00 19.20
	ATOM					486	39.245	53.051	89.927	1.00 15.13
	ATOM					487	43.455	56.279	85.089	1.00 34.97
	ATOM					487	44.032	57.092	84.070	1.00 38.06
6						487	43.491	56.622	82.758	1.00 43.55
	ATOM					487	42.951	55.537	82.604	1.00 46.30
	ATOM		СВ			487	45.591	57.038	84.085	1.00 43.93
	MOTA					487	46.196	58.169	83.302	1.00 56.10
	ATOM	3873	OD1	ASN	Α	487	46.057	58.189	82.077	1.00 42.12

	ATOM	3874	ND2	ASN A 48	7	46.829	59.112	84.007	1.00 65.62
	MOTA	3875	N	ALA A 48		43.662	57.435	81.781	1.00 39.34
	MOTA	3876	CA	ALA A 48		43.201	57.055	80.472	1.00 38.25
	ATOM	3877	С	ALA A 48		44.024	55.900	79.809	1.00 43.58
5	ATOM	3878	0	ALA A 48		43.596	55.317	78.834	1.00 44.11
	ATOM	3879	СВ	ALA A 48		43.153	58.314	79.621	1.00 37.54
	ATOM	3880	N	THR A 48		45.207	55.555	80.314	1.00 37.34
	ATOM	3881	CA	THR A 48		45.996	54.499	79.715	1.00 36.16
	ATOM	3882	С	THR A 48		45.270	53.181	79.792	1.00 45.74
10	ATOM	3883	0	THR A 48		45.476	52.233	79.057	1.00 47.78
,	ATOM	3884	СВ	THR A 48		47.296	54.458	80.503	1.00 31.01
	ATOM	3885	OG1			46.961	54.457	81.872	1.00 31.01
	ATOM	3886	CG2			47.993	55.771	80.229	1.00 33.33
	ATOM	3887	N	ASP A 49		44.337	53.182	80.708	1.00 26.26
15	ATOM	3888	CA	ASP A 49		43.560	52.018	80.972	1.00 40.75
	ATOM	3889	C	ASP A 49		42.759	51.515	79.786	1.00 51.49
	ATOM	3890	ŏ	ASP A 49		42.396	50.342	79.651	1.00 52.21
	ATOM	3891	СВ	ASP A 49		42.676	52.345	82.184	
	ATOM	3892	CG	ASP A 49		43.413	52.884	83.380	1.00 54.04 1.00 53.83
20	ATOM	3893		ASP A 49		44.621	52.777	83.616	
220	ATOM	3894		ASP A 49		42.565	53.446		1.00 62.93
	ATOM	3895	N	LEU A 49		42.486		84.165 78.938	1.00 35.66
	ATOM	3896		LEU A 49		41.752	52.450		1.00 42.42
	ATOM	3897	C	LEU A 49		42.712	52.250	77.723	1.00 43.54
25	ATOM	3898	Ö	LEU A 49			51.977	76.585	1.00 43.97
23	ATOM	3899	СВ	LEU A 49		42.340 40.984	51.438	75.588	1.00 42.53
	ATOM	3900	CG	LEU A 49			53.528	77.421	1.00 44.89
	ATOM	3901		LEU A 49		39.794	53.747	78.338	1.00 48.31
	ATOM	3902		LEU A 49		38.558	54.171	77.552	1.00 49.16
30	ATOM	3903	N N	LYS A 49		39.377	52.494	79.125	1.00 39.24
50	ATOM	3904	CA	LYS A 49		43.958	52.403	76.754	1.00 42.32
	ATOM	3905	C	LYS A 49		44.999	52.320	75.696	1.00 44.57
	ATOM	3906	Ö	LYS A 49		44.826	51.165	74.680	1.00 49.08
	ATOM	3907	СВ	LYS A 49		44.810	51.343	73.473	1.00 49.66
35	ATOM	3908	CG	LYS A 49		46.359	52.177	76.401	1.00 48.47
3,5	ATOM	3909	CD	LYS A 49		47.487	52.883	75.629	1.00 88.73
	ATOM	3910	CE	LYS A 49		48.852	52.537	76.197	1.00100.00
	ATOM	3911	NZ	LYS A 49		48.786 50.103	51.460	77.300	1.00100.00
	ATOM	3912	N	ASP A 49		44.711	50.896 49.917	77.541	1.00100.00
40	ATOM	3913	CA	ASP A 49		44.664	49.517	75.227	1.00 41.86
••	ATOM	3914	C	ASP A 49		43.220	48.162	74.372 74.215	1.00 40.17
	ATOM	3915	ŏ	ASP A 49		43.031	46.973	73.889	1.00 44.29 1.00 42.00
	ATOM	3916	СВ	ASP A 49		45.560	47.699	75.015	
	ATOM	3917	CG	ASP A 49		47.021	48.130	74.956	1.00 41.52
45	ATOM	3918		ASP A 49		47.467	48.451	73.856	1.00 67.01 1.00 77.10
	MOTA	3919	OD2	ASP A 49	3	47.678	48.131	75.984	1.00 77.10
	ATOM	3920	N	LEU A 49		42.193	49.005	74.475	1.00 37.19
	ATOM	3921	CA	LEU A 49		40.789	48.512	74.526	1.00 40.09
	ATOM	3922	С	LEU A 49		39.992	48.877	73.245	1.00 30.32
50	ATOM	3923	0	LEU A 49		39.897	50.029	72.863	1.00 37.70
	ATOM	3924	СВ	LEU A 49		40.098	49.125	75.733	1.00 30.93
	ATOM	3925	CG	LEU A 49		40.376	48.433	77.063	1.00 32.32
	ATOM	3926		LEU A 49		39.229	48.580	78.052	1.00 30.39
	ATOM	3927		LEU A 49		40.611	46.925	76.918	1.00 30.39
55	ATOM	3928	N	SER A 49		39.477	47.825	72.631	1.00 25.56
	ATOM	3929	CA	SER A 49		38.674	48.017	71.457	1.00 23.38
	ATOM	3930	C	SER A 49		37.344	48.670	71.856	1.00 22.23
	ATOM	3931	ō	SER A 49		36.968	48.706	73.038	1.00 31.27
	ATOM	3932	СВ	SER A 49		38.380	46.705	70.795	1.00 31.21
60	ATOM	3933	OG	SER A 49		37.192	46.143	71.317	
	ATOM	3934	N	SER A 49		36.627	49.184	70.865	1.00 33.60
	ATOM	3935	CA	SER A 49		35.363	49.104	71.139	1.00 29.48 1.00 26.67
	ATOM	3936	C	SER A 49		34.495	48.747	71.744	1.00 26.67
	ATOM	3937	0	SER A 49		33.744	48.960	72.697	1.00 29.34
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	ATOM	3938	CB	SER A 4	96	34.760	50.441	69.894	1.00 24.67
	ATOM	3939	OG	SER A 4		33.749	49.597	69.397	
	ATOM	3940	N	HIS A 4					1.00 48.80
						34.674	47.547	71.219	1.00 26.61
5	ATOM	3941	CA	HIS A 4		33.949	46.383	71.750	1.00 29.22
3	ATOM	3942	С	HIS A 4		34.156	46.148	73.275	1.00 37.24
	ATOM	3943	0	HIS A 4	97	33.238	45.863	74.041	1.00 38.21
	ATOM	3944	CB	HIS A 4	97	34.364	45.106	70.978	1.00 30.69
	ATOM	3945	CG	HIS A 4		34.182	45.348	69.545	
	ATOM	3946		HIS A 4		32.943	45.204		1.00 34.29
10	ATOM	3947		HIS A 4				68.962	1.00 35.42
10						35.054	45.833	68.622	1.00 36.68
	ATOM	3948		HIS A 4		33.075	45.531	67.702	1.00 35.05
	ATOM	3949	NE2	HIS A 4	.97	34.330	45.932	67.462	1.00 35.88
	MOTA	3950	N	GLN A 4	98	35.406	46.243	73.715	1.00 33.56
	ATOM	3951	CA	GLN A 4	98	35.737	46.008	75.094	1.00 29.69
15	ATOM	3952	С	GLN A 4		35.263	47.122	75.965	
	ATOM	3953	ō	GLN A 4		34.842			1.00 27.11
	ATOM	3954	CB				46.930	77.089	1.00 23.92
				GLN A 4		37.221	45.659	75.248	1.00 29.95
	ATOM	3955	CG	GLN A 4		37.582	44.317	74.544	1.00 25.78
- 00	MOTA	3956	CD	GLN A 4		39.074	44.084	74.535	1.00 28.64
20	ATOM	3957	OE1	GLN A 4	98	39.796	44.891	73.960	1.00 26.62
	ATOM	3958	NE2	GLN A 4	98	39.561	43.049	75.218	
	ATOM	3959	N	LEU A 4		35.289			1.00 20.96
	ATOM	3960	CA	LEU A 4			48.301	75.431	1.00 27.13
						34.819	49.396	76.229	1.00 29.32
25	ATOM	3961	С	LEU A 4		33.351	49.162	76.632	1.00 28.39
25	ATOM	3962	0	LEU A 4		32.893	49.361	77.780	1.00 29.41
	ATOM	3963	CB	LEU A 4	99	34.991	50.709	75.436	1.00 31.70
	ATOM	3964	CG	LEU A 4		36.242	51.512	75.788	1.00 39.76
	ATOM	3965	CD1			37.335	50.572	76.278	
	ATOM	3966	CD2			36.718			1.00 42.91
30	ATOM	3967					52.268	74.555	1.00 39.08
50			N	ASN A 5		32.606	48.737	75.642	1.00 15.23
	ATOM	3968	CA	ASN A 5		31.213	48.508	75.828	1.00 13.44
	ATOM	3969	С	ASN A 5	00	30.919	47.455	76.864	1.00 18.98
	ATOM	3970	0	ASN A 5	00	29.997	47.602	77.705	1.00 19.01
	ATOM	3971	CB	ASN A 5	00	30.604	48.129	74.476	1.00 12.21
35	ATOM	3972	CG	ASN A 5		29.093	48.214		
	ATOM	3973		ASN A 5				74.426	1.00 37.49
	ATOM	3974		ASN A 5		28.433	49.151	74.930	1.00 36.17
	ATOM	3975				28.542	47.218	73.787	1.00 18.34
			N	GLU A 5		31.699	46.366	76.743	1.00 14.20
40	ATOM	3976	CA	GLU A 5		31.626	45.224	77.625	1.00 13.27
40	ATOM	3977	С	GLU A 5	01	31.948	45.676	79.063	1.00 21.59
	ATOM	3978	0	GLU A 5	01	31.175	45.463	80.009	1.00 25.02
	ATOM	3979	CB	GLU A 5	01	32.446	44.057	77.053	1.00 14.95
	ATOM	3980	CG	GLU A 5		32.371	42.827	77.989	1.00 30.40
	ATOM	3981	CD	GLU A 5		30.946		78.199	
45	ATOM	3982		GLU A 5			42.399		1.00 39.28
	ATOM	3983				30.050	42.672	77.413	1.00 76.70
			OE2			30.780	41.694	79.292	1.00 46.10
	ATOM	3984	N	PHE A 5		33.059	46.400	79.226	1.00 18.07
	MOTA	3985	CA	PHE A 5		33.395	46.952	80.530	1.00 21.54
	ATOM	3986	С	PHE A 5	02	32.179	47.679	81.125	1.00 23.38
50	ATOM	3987	0	PHE A 5	02	31.786	47.491	82.301	1.00 21.47
	ATOM	3988	CB	PHE A 5		34.507	48.012		
	ATOM	3989	CG	PHE A 5				80.327	1.00 26.05
	ATOM	3990		DUE A C	02	34.590	49.082	81.393	1.00 30.41
			CDI	PHE A 5	02	35.085	48.781	82.662	1.00 29.68
55	ATOM	3991		PHE A 5		34.211	50.402	81.132	1.00 39.16
<i>55</i> .	ATOM	3992	CE1	PHE A 5	02	35.183	49.773	83.638	1.00 31.12
	ATOM	3993	CE2	PHE A 5	02	34.305	51.414	82.096	1.00 40.46
	ATOM	3994	CZ	PHE A 5		34.812	51.090	83.352	
	ATOM	3995	N	LEU A 5					1.00 35.41
	ATOM	3996	CA			31.613	48.557	80.288	1.00 18.39
60	ATOM			LEU A 5		30.487	49.343	80.692	1.00 22.78
00		3997	C	LEU A 5		29.337	48.491	81.178	1.00 31.04
	ATOM	3998	0	LEU A 5		28.768	48.784	82.243	1.00 29.23
	ATOM	3999	CB	LEU A 5		30.002	50.325	79.619	1.00 24.68
	ATOM	4000	CG	LEU A 5	03	30.888	51.571	79.465	1.00 27.47
	MOTA	4001	CD1	LEU A 5		30.415	52.376	78.259	1.00 24.86
						-			23.00

	MOTA	4002	CD2	LEU A	503	30.860	52.420	80.733	1.00 20.54
	ATOM	4003	N	ALA A	504	29.012	47.444	80.378	1.00 27.79
	ATOM	4004	CA	ALA A					
						27.911	46.474	80.643	1.00 24.63
_	MOTA	4005	С	ALA A	504	28.140	45.752	81.939	1.00 27.71
5	ATOM	4006	0	ALA A	504	27.265	45.577	82.817	1.00 28.62
	ATOM	4007	CB	ALA A	504	27.762	45.482	79.496	
									1.00 23.87
	ATOM	4008	N	GLN A		29.382	45.344	82.066	1.00 22.16
	MOTA	4009	CA	GLN A	505	29.738	44.710	83.299	1.00 21.02
	ATOM	4010	С	GLN A	505	29.489	45.737	84.423	1.00 31.26
10	ATOM	4011	Ö	GLN A					
. 10						28.787	45.507	85.413	1.00 32.31
	ATOM	4012	CB	GLN A		31.202	44.209	83.270	1.00 18.95
	MOTA	4013	CG	GLN A	505	31.367	42.881	82.495	1.00 13.72
	ATOM	4014	CD	GLN A	505	32.806	42.549	82.136	1.00 31.75
	ATOM	4015		GLN A					
15						33.796	42.969	82.768	1.00 43.14
15	ATOM	4016	NE2	GLN A		32.923	41.781	81.085	1.00 39.34
	ATOM	4017	N	THR A	506	30.056	46.918	84.263	1.00 25.95
	ATOM	4018	CA	THR A		29.855	47.864	85.302	
TT en									1.00 23.64
	ATOM	4019	C	THR A		28.411	48.101	85.579	1.00 23.89
. (M)	MOTA	4020	0	THR A	506	27.923	47.999	86.696	1.00 22.75
20	ATOM	4021	CB	THR A	506	30.600	49.130	85.008	1.00 23.72
	ATOM	4022	OG1						
je 4.						31.938	48.749	84.742	1.00 27.18
9 9 833	MOTA	4023	CG2	THR A		30.502	49.961	86.260	1.00 11.12
migrack	MOTA	4024	N	LEU A	507	27.727	48.408	84.518	1.00 17.92
150 207	ATOM	4025	CA	LEU A	507	26.334	48.683	84.604	1.00 17.22
25	ATOM	4026	С	LEU A					
4.						25.618	47.683	85.442	1.00 25.65
j= 40	ATOM	4027	0	LEU A	507	24.816	48.073	86.266	1.00 27.85
	ATOM	4028	CB	LEU A	507	25.693	48.686	83.224	1.00 17.85
\$	ATOM	4029	CG	LEU A		24.207	48.930		
]=4 <u>,</u>			CD1					83.336	1.00 21.02
30	ATOM	4030		LEU A		23.974	50.290	83.970	1.00 22.48
30	MOTA	4031	CD2	LEU A	507	23.599	48.919	81.949	1.00 15.25
	ATOM	4032	N	GLN A	508	25.878	46.395	85.194	1.00 21.35
	ATOM	4033	CA	GLN A		25.215	45.333		
'इन सारे .com								85.979	1.00 18.08
	ATOM	4034	С	GLN A		25.386	45.561	87.508	1.00 34.24
8 8	ATOM	4035	0	GLN A	508	24.653	45.017	88.343	1.00 34.04
35	MOTA	4036	CB	GLN A	508	25.713	43.917	85.608	1.00 10.94
•	MOTA	4037	CG	GLN A		25.366			
							43.446	84.191	1.00 26.42
	ATOM	4038	CD	GLN A		25.635	41.944	84.002	1.00 52.93
	ATOM	4039	OE1	GLN A		26.550	41.396	84.628	1.00 32.89
	ATOM	4040	NE2	GLN A	508	24.864	41.252	83.147	1.00 34.36
40	ATOM	4041	N	ARG A		26.380	46.361		
••								87.901	1.00 33.73
	MOTA	4042	CA	ARG A		26.600	46.614	89.328	1.00 32.53
	ATOM	4043	С	ARG A	509	26.153	48.016	89.727	1.00 33.63
	MOTA	4044	0	ARG A	509	26.509	48.522	90.777	1.00 31.08
	ATOM	4045	CB	ARG A	509	28.055	46.440		
45								89.760	1.00 29.22
7.7	ATOM	4046	CG	ARG A		28.553	45.014	89.733	1.00 29.78
	MOTA	4047	CD	ARG A	509	27.744	44.054	90.609	1.00 30.86
,	ATOM	4048	NE	ARG A	509	28.533	43.602	91.756	1.00 82.23
	ATOM	4049	CZ	ARG A		29.842	43.274	91.726	1.00100.00
	ATOM	4050		ARG A					
50						30.579	43.315	90.613	1.00 92.85
30	MOTA	4051	NH2	ARG A	509	30.430	42.881	92.855	1.00 91.85
	MOTA	4052	N	ALA A	510	25.384	48.659	88.880	1.00 32.59
	ATOM	4053	CA	ALA A	510	24.952	49.985	89.215	1.00 32.51
	ATOM	4054	C	ALA A					
						24.151	49.845	90.479	1.00 34.97
	ATOM	4055	0	ALA A		23.601	48.785	90.693	1.00 37.57
55	ATOM	4056	CB	ALA A	510	24.189	50.622	88.063	1.00 32.91
	ATOM	4057	N	PRO A		24.174	50.856	91.334	
	MOTA	4058							1.00 25.14
			CA	PRO A		24.867	52.102	91.052	1.00 21.00
	ATOM	4059	С	PRO A	511	26.217	52.178	91.694	1.00 29.23
	ATOM	4060	0	PRO A	511	26.445	51.601	92.723	1.00 28.16
60	ATOM	4061	CB	PRO A		24.102	53.169	91.818	
	ATOM	4062	CG						1.00 21.55
. 1				PRO A		23.316	52.432	92.886	1.00 28.68
	ATOM	4063	CD	PRO A		23.169	50.995	92.407	1.00 25.16
	MOTA	4064	N	LEU A	512	27.094	52.968	91.109	1.00 32.95
	ATOM	4065	CA	LEU A		28.394	53.188	91.686	
						20.554	,55,100	21.000	1.00 33.42

	ATOM	4066	С	LEU A	512	28.287	54.512	00 207	2 00	20 65
	ATOM	4067	ŏ	LEU A				92.397		38.65
	ATOM	4068				27.388	55.305	92.114		40.69
			CB	LEU A		29.453	53.350	90.587	1.00	34.40
_	ATOM	4069	CG	LEU A		30.178	52.049	90.216	1.00	40.13
5	ATOM	4070	CD1			29.222	51.086	89.508		39.04
	MOTA	4071	CD2	LEU A	512	31.322	52.385	89.273		44.61
	ATOM	4072	N	PRO A		29.196	54.781	93.312		31.05
	ATOM	4073	CA	PRO A		29.167				
		4074	C				56.058	94.008		27.16
10	ATOM			PRO A		29.296	57.203	93.019	1.00	23.76
10	ATOM	4075	0	PRO A		30.121	57.182	92.118	1.00	27.17
	ATOM	4076	CB	PRO A	513	30.387	56.013	94.948	1.00	25.59
	ATOM	4077	CG	PRO A	513	30.702	54.542	95.149		27.14
	ATOM	4078	CD	PRO A	513	30.030	53.779	94.032		25.00
	ATOM	4079	N	LEU A		28.478	58.203	93.185		
15	ATOM	4080	CA	LEU A						22.92
1.0						28.516	59.350	92.279		27.55
	MOTA	4081	C	LEU A		29.930	59.766	91.940	1.00	31.95
	MOTA	4082	0	LEU A		30.287	59.908	90.765	1.00	37.11
	ATOM	4083	CB	LEU A	514	27.673	60.564	92.741		30.03
398 ₆	ATOM	4084	CG	LEU A	514	27.428	61.626	91.648	1.00	
20	ATOM	4085	CD1	LEU A		26.648	61.082	90.440		
43 20	ATOM	4086		LEU A		26.699	62.780		1.00	
ļ.	ATOM							92.272	1.00	
· · · · · · · ·		4087	N	GLY A		30.731	59.989	92.979	1.00	
	ATOM	4088	CA	GLY A		32.131	60.384	92.811	1.00	25.59
	ATOM	4089	С	GLY A		32.902	59.472	91.835	1.00	33.83
25	ATOM	4090	0	GLY A	515	33.746	59.914	91.035	1.00	
ial.	ATOM	4091	N	HIS A		32.602	58.180	91.891	1.00	
Berris	ATOM	4092	CA	HIS A		33.257	57.255			
#	ATOM	4093	C	HIS A				90.998	1.00	
ils ils						32.911	57.578	89.560	1.00	27.62
7. 30	ATOM	4094	0	HIS A		33.786	57.596	88.695	1.00	28.67
	ATOM	4095	CB	HIS A	516	32.826	55.814	91.282	1.00	25.39
n.	ATOM	4096	CG	HIS A		33.452	55.283	92.505	1.00	
12 H	ATOM	4097	ND1	HIS A	516	33.635	56.092	93.602	1.00	
Residence deserving	ATOM	4098		HIS A		33.929	54.037	92.791		
12 m	ATOM	4099		HIS A		34.205			1.00	
¹ 35	ATOM	4100					55.336	94.534	1.00	
22				HIS A		34.390	54.099	94.085	1.00	
	ATOM	4101	N	ILE A		31.617	57.815	89.315	1.00	21.40
	MOTA	4102	CA	ILE A		31.137	58.107	87.973	1.00	22.75
	ATOM	4103	С	ILE A	517	31.706	59.424	87.462	1.00	
	ATOM	4104	0	ILE A	517	32.246	59.558	86.352	1.00	
40	ATOM	4105	CB	ILE A		29.601	58.024	87.930	1.00	
	ATOM	4106	CG1	ILE A		29.225	56.610			
	ATOM	4107	CG2					88.312	1.00	
	ATOM	4108		ILE A		29.013	58.285	86.536	1.00	
						29.305	55.665	87.105	1.00	
15	ATOM	4109	N	LYS A		31.589	60.416	88.308	1.00	27.28
45	ATOM	4110	CA	LYS A		32.108	61.690	87.955	1.00	
* * .	ATOM	4111	С	LYS A		33.558	61.482	87.485	1.00	
	ATOM	4112	0	LYS A	518	33.982	61.831	86.391	1.00	
	ATOM	4113	CB	LYS A		32.038	62.557	89.210	1.00	
	ATOM	4114	CG	LYS A		30.641	63.060	89.591		
50	ATOM	4115	CD	LYS A					1.00	
		4116				30.721	64.276	90.537	1.00	
	ATOM		CE	LYS A		29.379	64.877	90.962	1.00	37.11
	ATOM	4117	NZ	LYS A		28.924	65.988	90.104	1.00	52.30
	MOTA	4118	N	ARG A	519	34.322	60.899	88.361	1.00	
	MOTA	4119	CA	ARG A	519	35.703	60.636	88.098	1.00	
55	MOTA	4120	С	ARG A		35.862	59.874	86.802	1.00	
	ATOM	4121	Ō	ARG A		36.812	60.084			
	ATOM	4122	CB	ARG A				86.051	1.00	
						36.313	59.844	89.276	1.00	
	ATOM	4123	CG	ARG A		37.721	59.308	89.036	1.00	
60	ATOM	4124	CD	ARG A		38.668	60.320	88.404	1.00	
60	ATOM	4125	NE	ARG A		40.086	60.008	88.616	1.00	
	ATOM	4126	CZ	ARG A	519	41.076	60.858	88.349	1.00	
	ATOM	4127		ARG A		40.838	62.073	87.880	1.00	
	ATOM	4128		ARG A		42.329	60.486			
	ATOM	4129	N	MET A				88.543	1.00	
	7.12 OF1	2142	14	THE A	J20	34.937	58.956	86.565	1.00	25.08

	MOTA	4130	CA	MET A 5	20	34.979	58.121	85.379	1.00	24.56
	ATOM	4131	С	MET A 5		34.906	58.918	84.086		29.37
	MOTA	4132	0	MET A 5		35.651	58.687	83.114		27.92
	ATOM	4133	CB	MET A 5		33.905	57.007	85.442	1.00	26.98
5	ATOM	4134	CG	MET A 5	520	34.082	55.902	84.399	1.00	28.02
	MOTA	4135	SD	MET A 5	520	32.830	54.591	84.479	1.00	27.87
	ATOM	4136	CE	MET A 5		33.246	53.825	86.070		
										22.09
	MOTA	4137	N	GLN A 5		33.982	59.864	84.067	1.00	28.32
	MOTA	4138	CA	GLN A 5	521	33.838	60.672	82.886	1.00	28.34
10	ATOM	4139	С	GLN A 5	521	35.067	61.540	82.785		36.52
-0	MOTA	4140	Ö	GLN A 5		35.514	61.879	81.707		
										35.87
	ATOM	4141	CB	GLN A 5		32.514	61.451	82.863	1.00	28.34
	MOTA	4142	CG	GLN A 5	521	32.564	62.774	82.079	1.00	9.68
	MOTA	4143	CD	GLN A 5		32.890	62.572	80.616	1 00	27.55
15		4144		GLN A 5		33.382				
13	ATOM						63.491	79.924		28.25
	MOTA	4145	NE2	GLN A 5	21	32.657	61.368	80.142	1.00	25.70
	MOTA	4146	N	GLU A 5	522	35.626	61.827	83.963	1.00	36.19
	ATOM	4147	CA	GLU A 5	522	36.818	62.648	84.171		36.13
	ATOM	4148	C	GLU A 5		38.136	62.046			
20								83.662		42.48
20	MOTA	4149	0	GLU A 5		39.099	62.735	83.335	1.00	42.40
	ATOM	4150	CB	GLU A 5	522	36.857	63.035	85.641	1.00	37.79
	MOTA	4151	CG	GLU A S		38.233	63.196	86.273		58.85
	ATOM	4152	CD	GLU A S		38.046	64.040	87.493		73.64
	ATOM	4153	OE1	GLU A S	522	37.006	64.641	87.709	1.00	45.66
25	MOTA	4154	OE2	GLU A S	522	39.081	64.037	88.289	1.00	47.91
	ATOM	4155	N	VAL A		38.188	60.739	83.552		40.13
	ATOM	4156	CA	VAL A		39.401	60.136	83.058		37.49
	ATOM	4157	С	VAL A S	523	39.205	59.351	81.778	1.00	38.88
	ATOM	4158	0	VAL A S	523	40.195	59.016	81.138	1.00	40.21
30	ATOM	4159	CB	VAL A S	523	40.184	59.370	84.102		40.01
		4160								
	ATOM			VAL A		40.231	60.165	85.413		39.12
	MOTA	4161	CG2	VAL A	523	39.534	58.017	84.320	1.00	39.82
	MOTA	4162	N	TYR A S	524	37.952	59.048	81.379	1.00	30.35
	ATOM	4163	CA	TYR A S		37.801	58.330	80.114		28.11
35										
35	ATOM	4164	C	TYR A		37.061	59.144	79.074		33.14
	MOTA	4165	0	TYR A S	524	37.076	58.802	77.908	1.00	35.84
	ATOM	4166	CB	TYR A	524	37.281	56.878	80.119	1.00	25.56
	ATOM	4167	CG	TYR A		37.941	55.960	81.111		20.87
	ATOM	4168		TYR A		39.324	55.938			
40								81.258		21.59
40	ATOM	4169		TYR A		37.170	55.083	81.879		19.80
	MOTA	4170	CE1	TYR A	524	39.905	55.063	82.176	1.00	25.64
	MOTA	4171	CE2	TYR A !	524	37.731	54.227	82.827	1.00	18.61
	ATOM	4172	CZ	TYR A		39.116	54.231	82.969		19.81
4.5	MOTA	4173	OH	TYR A		39.706	53.402	83.863	1.00	23.92
45	ATOM	4174	N	ASN A	525	36.416	60.221	79.496	1.00	25.98
	ATOM	4175	CA	ASN A	525	35.687	61.088	78.588	1.00	25.01
	ATOM	4176	С	ASN A		34.661	60.354	77.735		29.86
				ASN A						
	ATOM	4177	0_			34.533	60.535	76.499		29.39
	MOTA	4178	CB	ASN A		36.637	61.922	77.739		29.55
50	MOTA	4179	CG	ASN A	525	35.949	62.980	76.894	1.00	30.32
	ATOM	4180	OD1	ASN A	525	36.460	63.332	75.850		32.77
	MOTA	4181		ASN A		34.822	63.527	77.344		
										13.80
	ATOM	4182	N	PHE A		33.924	59.512	78.436		24.21
	ATOM	4183	CA	PHE A	526	32.900	58.745	77.807	1.00	25.14
55	ATOM	4184	С	PHE A	526	31.846	59.631	77.214		31.74
	ATOM	4185	Ö	PHE A		31.161	59.241	76.272		
										34.99
	ATOM	4186	CB	PHE A		32.256	57.732	78.781	1.00	26.60
	ATOM	4187	CG	PHE A	526	33.115	56.499	78.978	1.00	23.82
	ATOM	4188	CDI	PHE A		34.017	56.080	78.000		25.00
60	ATOM	4189		PHE A		33.031	55.767			
.00								80.159		21.74
	ATOM	4190		PHE A		34.783	54.927	78.173		27.63
	ATOM	4191	CE2	PHE A	526	33.817	54.634	80.370	1.00	25.42
	MOTA	4192	CZ	PHE A		34.683	54.202	79.364		25.28
	ATOM	4193	N	ASN A		31.689	60.815	77.760		28.22
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		MOTA	4194	CA	ASN A		30.657	61.688	77.214	1.00	31.18
		ATOM	4195	С	ASN A	527	30.884	62.046	75.744	1.00	33.17
		ATOM	4196	0	ASN A	527	29.965	62.394	74.999	1.00	30.80
		ATOM	4197	CB	ASN A		30.479	62.967	78.052		36.41
	5	ATOM	4198	CG	ASN A		29.638	62.752	79.292		46.99
			4199		ASN A						
		MOTA					29.647	63.571	80.209		36.82
		ATOM	4200		ASN A		28.922	61.636	79.338		43.55
		MOTA	4201	N	ALA A	528	32.136	61.947	75.348	1.00	27.46
		MOTA	4202	CA	ALA A	528	32.581	62.278	74.005	1.00	26.48
	10	MOTA	4203	С	ALA A	528	32.335	61.188	72.950		32.09
		MOTA	4204	0	ALA A		32.420	61.404	71.753		32.09
		MOTA	4205	CB	ALA A		34.076	62.584	74.105		26.04
		MOTA	4206	N	ILE A		32.067	59.983	73.402		31.35
		ATOM	4207	CA	ILE A		31.854	58.859	72.529	1.00	28.47
	15	ATOM	4208	C	ILE A	529	30.492	58.904	71.887	1.00	35.96
		ATOM	4209	0	ILE A	529	29.486	59.023	72.578		38.79
		ATOM	4210	СВ	ILE A		32.103	57.544	73.264		30.17
			4211	CG1							
		ATOM					33.622	57.291	73.392		31.37
	20	ATOM	4212		ILE A		31.428	56.411	72.489		27.63
	20	MOTA	4213	CD1	ILE A	529	34.059	56.515	74.635	1.00	33.41
₹\$#¥₹ 		ATOM	4214	N	ASN A	530	30.462	58.806	70.559		34.86
4D		ATOM	4215	CA	ASN A	530	29.196	58.841	69.852		36.44
1		ATOM	4216	С	ASN A		28.596	57.495	69.473		39.90
140. 240.	100				ASN A						
19 and	25	ATOM	4217	0			27.452	57.437	69.043		41.37
eja:	25	ATOM	4218	CB	ASN A		28.951	60.044	68.928		51.44
H.		ATOM	4219	CG	ASN A	530	28.461	61.253	69.732	1.001	100.00
ļ-4.		MOTA	4220	OD1	ASN A	530	27.652	61.109	70.665	1.001	100.00
		MOTA	4221	ND2	ASN A	530	28.955	62,442	69.392		91.39
##		MOTA	4222	N	ASN A		29.368	56.403	69.688		30.37
H	30	MOTA	4223	CA	ASN A		28.912				
n.	30							55.030	69.446		28.14
1822 15 13 12 15 13 15 15 15 15 15 15 15 15 15 15 15 15 15 1		MOTA	4224	С	ASN A		27.696	54.753	70.360		32.80
$\Pi_{\mathbf{k}}$		MOTA	4225	0	ASN A		27.746	54.887	71.611		36.74
		ATOM	4226	CB	ASN A	531	30,092	54.066	69.690	1.00	24.31
##.		ATOM	4227	CG	ASN A	531	29.770	52.601	69.730	1.00	34.44
12 H	35	ATOM	4228	OD1	ASN A	531	28.795	52.182	70.359		36.49
-4		ATOM	4229		ASN A		30.643	51.810	69.099		30.57
		ATOM	4230	N	SER A		26.570	54.403			
									69.734		22.02
		MOTA	4231	CA	SER A		25.325	54.183	70.459		19.67
	40	ATOM	4232	С	SER A		25.323	53.208	71.627		26.15
	40	ATOM	4233	0	SER A	532	24.767	53.475	72.680	1.00	26.64
		MOTA	4234	CB	SER A	532	24.090	54.034	69.582		26.92
		ATOM	4235	OG	SER A	532	24.294	53.211	68.452		23.59
		ATOM	4236	N	GLU A		25.929	52.062	71.423		22.68
		ATOM	4237	CA	GLU A						
	45		4237	CA	GLU A		25.995	51.036	72.420		22.97
	43	ATOM					26.677	51.569	73.635		30.48
		MOTA	4239	0	GLU A		26.125	51.539	74.749		31.13
		MOTA	4240	CB	GLU A		26.683	49.779	71.850	1.00	23.96
		MOTA	4241	CG	GLU A	533	25.827	49.146	70.733		20.82
		MOTA	4242	CD	GLU A		24.611	48.450	71.276		40.65
	50	ATOM	4243		GLU A		24.432	48.256	72.476		36.25
		ATOM	4244		GLU A		23.782	48.038			
									70.339		25.87
		ATOM	4245	N	ILE A		27.872	52.101	73.392	1.00	26.20
		ATOM	4246	CA	ILE A		28.622	52.672	74.484	1.00	26.32
		ATOM	4247	С	ILE A	534	27.900	53.849	75.121	1.00	27.83
	<i>55</i>	ATOM	4248	0	ILE A	534	27.697	53.911	76.326		26.54
		ATOM	4249	CB	ILE A		30.051	53.022	74.102	1.00	29.16
		ATOM	4250		ILE A		30.738	51.808	73.479		
			4251								29.47
		MOTA			ILE A		30.801	53.458	75.353		28.28
	C0	MOTA	4252		ILE A		32.038	52.184	72.765	1.00	34.99
	60	ATOM	4253	N	ARG A		27.480	54.805	74.320	1.00	24.30
		MOTA	4254	CA	ARG A	535	26.804	55.898	74.949		22.51
		ATOM	4255	C	ARG A		25.573	55.401	75.701		28.19
		ATOM	4256	0	ARG A		25.212	55.808	76.791		32.61
		MOTA	4257	CB	ARG A		26.457	56.942	73.913		24.83
								JU. J34	, , , , , , ,	****	62.03

	ATOM	4258	CG	ARG A	A 535		25.970	58.229	74.541	1 00	21.49
	ATOM	4259	CD	ARG A			25.327	59.183	73.554		13.79
	MOTA	4260	NE	ARG A			25.194	60.457	74.213		31.38
	MOTA	4261	CZ	ARG A			26.256	61.140	74.554		29.41
5	ATOM	4262		ARG A			27.463	60.677	74.259		26.45
	ATOM	4263		ARG A			26.110	62.302	75.195		
	ATOM	4264	N	PHE A		_	24.911	54.466	75.126		19.99
	ATOM	4265	CA	PHE A			23.740	53.980			23.44
	ATOM	4266	C	PHE A			23.976	53.555	75.770		22.05
10	ATOM	4267	ō	PHE A			23.349	54.113	77.199		22.74
	ATOM	4268	CB	PHE A			23.117		78.105	1.00	22.06
	ATOM	4269	CG	PHE A			22.040	52.865	74.919		23.17
	ATOM	4270		PHE A			20.933	52.153	75.658		21.92
	ATOM	4271		PHE A				52.845	76.150		22.66
15	ATOM	4272		PHE A			22.145	50.783	75.882		23.25
10	ATOM	4273	CE2	PHE A			19.926	52.181	76.847		21.23
	ATOM	4274	CZ	PHE A			21.147	50.101	76.576		24.70
	ATOM	4275					20.047	50.811	77.065	1.00	20.57
			N	ARG A			24.863	52.560	77.364		18.22
20	ATOM	4276	CA	ARG A			25.239	51.995	78.665	1.00	19.20
20	ATOM	4277	C	ARG A		•	25.932	52.963	79.618	1.00	27.62
	ATOM	4278	0	ARG A			25.803	52.845	80.837	1.00	26.73
	ATOM	4279	CB	ARG A			26.035	50.709	78.556	1.00	18.91
	ATOM	4280	CG	ARG A			25.318	49.656	77.708		16.55
25	ATOM	4281	CD	ARG A	537		26.181	48.426	77.387		21.58
25	ATOM	4282	NE	ARG A	537		25.341	47.357	76.886		28.42
	ATOM	4283	CZ	ARG A			25.060	47.206	75.609		18.29
	ATOM	4284	NH1	ARG A	537		25.569	48.004	74.703		22.46
	ATOM	4285	NH2	ARG A	537		24.240	46.236	75.224		25.22
	ATOM	4286	N	TRP A	538		26.668	53.930	79.064		24.21
30	ATOM	4287	CA	TRP A	538		27.337	54.918	79.867		22.11
	MOTA	4288	С	TRP A	538		26.274	55.719	80.550		28.09
	ATOM	4289	0	TRP A	538		26.320	55.951	81.741		27.39
	ATOM	4290	CB	TRP A			28.064	55.888	78.949		20.48
	ATOM	4291	CG	TRP A			28.606	57.157	79.580		21.29
35	ATOM	4292	CD1	TRP A			28.641	58.345	78.968		22.86
	MOTA	4293		TRP A			29.286	57.352	80.845		21.79
	ATOM	4294	NE1				29.228	59.270	79.769		22.70
	ATOM	4295	CE2	TRP A			29.643	58.696	80.911		24.79
	ATOM	4296		TRP A			29.574	56.535	81.946		23.35
40	ATOM	4297		TRP A			30.280	59.248	82.025		25.89
	ATOM	4298		TRP A			30.203	57.056	83.046		
	ATOM	4299	CH2	TRP A			30.562	58.405	83.081		23.35
	MOTA	4300	N	LEU A			25.303	56.161	79.758		24.89
	ATOM	4301	CA	LEU A			24.229	56.974			27.31
45	ATOM	4302	c	LEU A			23.369	56.245	80.306		27.18
	ATOM	4303	ō	LEU A			22.857	56.822	81.332		28.25
	ATOM	4304	СВ	LEU A			23.428		82.266		27.19
	ATOM	4305	CG	LEU A			24.269	57.812 58.682	79.262		26.37
	ATOM	4306		LEU A					78.279		25.71
50	ATOM	4307		LEU A			23.369	59.424	77.290		21.79
	ATOM	4308		ARG A			25.146	59.680	79.011		23.51
	ATOM	4309		ARG A			23.199	54.960	81.188		27.56
	ATOM	4310		ARG A			22.390	54.283	82.170		26.88
	ATOM	4311		ARG A			23.145	54.229	83.453		31.82
55	ATOM	4312					22.618	54.448	84.539		32.72
	ATOM	4313		ARG A			22.034	52.888	81.732		24.48
	MOTA			ARG A			21.447	52.885	80.331		32.96
		4314		ARG A			20.695	51.597	80.090	1.00	33.19
	MOTA	4315		ARG A			19.660	51.414	81.085		33.95
60	ATOM	4316		ARG A			19.151	50.242	81.409		30.83
.00	ATOM	4317		ARG A			19.564	49.132	80.849		25.37
	ATOM	4318		ARG A			18.186	50.186	82.317		30.30
	ATOM	4319		LEU A			24.414	53.948	83.318		28.93
	ATOM	4320		LEU A			25.239	53.895	84.505		26.36
	MOTA	4321	С	LEU A	541		25.036	55.210	85.277		31.00

		ATOM	4322	0	LEU A	5.43	24.632	55.246	86.439	1.00 31.62
		ATOM	4323	СВ	LEU A		26.702	53.586	84.094	1.00 31.02
		ATOM	4324	CG	LEU A		27.730	53.533	85.212	1.00 23.61
		ATOM	4325		LEU A		27.730	52.411	86.190	1.00 24.07
	5	ATOM	4326		LEU A		29.098	53.245	84.621	1.00 23.02
	,	ATOM	4327	N	CYS A		25.254	56.307	84.570	1.00 30.52
		ATOM	4328	CA	CYS A		25.234	57.661	85.105	1.00 30.32
		ATOM	4329	C	CYS A		23.808	57.996	85.805	1.00 31.70
		ATOM	4330	0	CYS A		23.801	58.536	86.914	1.00 32.71
	10	MOTA	4331	CB	CYS A		25.461	58.744	84.073	
	10		4331	SG	CYS A		27.085	58.488		1.00 31.30 1.00 34.39
		MOTA MOTA	4333	N	ILE A		22.711	57.708	83.347 85.125	1.00 34.39
			4334	CA						
		ATOM	4334		ILE A		21.382	57.982	85.643	1.00 23.12
	15	ATOM	4336	С 0	ILE A		21.199	57.161	86.885	1.00 30.15
	13	ATOM	4337	СВ	ILE A		20.900	57.645	87.972	1.00 30.73
		ATOM		CG1			20.340	57.627	84.585	1.00 23.75
		ATOM	4338		ILE A		20.369	58.664	83.468	1.00 24.09
en etc.		ATOM	4339				18.955	57.572	85.182	1.00 22.99
	20	ATOM	4340		ILE A		20.386	60.109	83.982	1.00 27.34
	20	ATOM	4341	N	GLN A		21.440	55.884	86.695	1.00 27.99
भूती विक्रमी		ATOM	4342	CA	GLN A		21.320	54.929	87.756	1.00 25.72
ļ=#s		MOTA	4343	С	GLN A		22.243	55.269	88.901	1.00 26.34
1 STR.		ATOM	4344	0	GLN A		22.029	54.826	90.014	1.00 26.24
	25	ATOM	4345	СВ	GLN A	-	21.562	53.512	87.210	1.00 26.76
499 BW	25	ATOM	4346	CG	GLN A		20.355	52.955	86.432	1.00 17.74
		ATOM	4347	CD	GLN A		20.598	51.604	85.743	1.00 32.62
#=#×		MOTA	4348	OE1	GLN A		20.326	51.432	84.551	1.00 38.66
S E		ATOM	4349		GLN A		21.063	50.627	86.494	1.00 14.93
il-A	20	ATOM	4350	N	SER A		23.286	56.033	88.625	1.00 21.73
- A - A - A - A - A - A - A - A - A - A	30	MOTA	4351	CA	SER A		24.187	56.392	89.685	1.00 22.42
# '##: ## 33		ATOM	4352	С	SER A		23.819	57.726	90.287	1.00 33.67
		ATOM	4353	0	SER A		24.567	58.257	91.133	1.00 37.22
		ATOM	4354	CB	SER A		25.646	56.322	89.338	1.00 21.57
12.0	0.5	ATOM	4355	OG	SER A			~54 . 968	89.163	1.00 31.72
L.	35	ATOM	4356	N	LYS A		22.662	58.251	89.841	1.00 23.09
-"		ATOM	4357	CA	LYS A		22.135	59.490	90.356	1.00 20.79
		MOTA	4358	С	LYS A		22.887	60.738	89.961	1.00 27.55
		MOTA	4359	0	LYS A		23.001	61.655	90.771	1.00 27.95
	40	ATOM	4360	CB	LYS A		22.126	59.449	91.881	1.00 21.71
	40	ATOM	4361	CG	LYS A		21.498	58.195	92.484	1.00 15.90
		MOTA	4362	CD	LYS A		20.245	57.814	91.731	1.00 39.84
		MOTA	4363	CE	LYS A		19.355	56.850	92.498	1.00 45.16
		ATOM	4364	NZ	LYS A		18.197	56.399	91.704	1.00 40.14
	45	ATOM	4365	N	TRP A		23.414	60.776	88.753	1.00 23.26
	43	ATOM	4366	CA	TRP A		24.141	61.931	88.289	1.00 21.90
		MOTA	4367	C	TRP A		23.221	62.901	87.570	1.00 29.82
		ATOM	4368	0	TRP A		`22.808	62.679	86.432	1.00 34.91
		ATOM	4369	CB	TRP A		25.262	61.500	87.361	1.00 21.04
	£Ω	MOTA	4370	CG	TRP A		26.254	62.591	87.206	1.00 22.57
	50	ATOM	4371		TRP A		26.224	63.769	87.844	1.00 25.87
		ATOM	4372		TRP A		27.437	62.588	86.417	1.00 23.40
		ATOM	4373		TRP A		27.316	64.511	87.517	1.00 25.64
		ATOM	4374		TRP A		28.081	63.819	86.635	1.00 27.46
	55	ATOM	4375		TRP A		28.014	61.668	85.547	1.00 26.21
	55	ATOM	4376		TRP A		29.279	64.162	85.995	1.00 27.44
		ATOM	4377		TRP A		29.195	62.009	84.923	1.00 28.70
		MOTA	4378		TRP A		29.822	63.236	85.138	1.00 28.41
		ATOM	4379	N	GLU A		22.888	63.995	88.227	1.00 22.95
	60	ATOM	4380	CA	GLU A		21.979	64.970	87.649	1.00 20.70
	60	ATOM	4381	C	GLU A		22.419	65.473	86.305	1.00 28.32
		ATOM	4382	0	GLU A		21.598	65.735	85.391	1.00 29.41
		ATOM	4383	CB	GLU A		21.635	66.144	88.607	1.00 22.45
		ATOM	4384	CG	GLU A		20.884	65.709	89.919	1.00 30.56
		ATOM	4385	CD	GLU A	. 548	20.337	66.848	90.765	1.00 59.35

	ATOM	4386	OE1	GLU A 54	8	20.336	68.021	90.413	1.00	81.52
	ATOM	4387		GLU A 54		19.888	66.450			
								91.925		57.05
	ATOM	4388	N	ASP A 54	9	23.728	65.661	86.201	1.00	24.72
	ATOM	4389	CA	ASP A 54	۵	24.276	66.190	84.981	1 00	21.48
<u>_</u> '										
5	ATOM	4390	С	ASP A 54	9	23.914	65.359	83.795	1.00	30.08
	MOTA	4391	0	ASP A 54	Q	23.760	65.869	82.697		32.05
	ATOM	4392	CB	ASP A 54	9	25.775	66.480	85.048	1.00	21.28
	MOTA	4393	CG	ASP A 54	Q.	26.076	67.463	86.130		37.74
	MOTA	4394		ASP A 54		25.432	68.479	86.297	1.00	48.21
10	ATOM	4395	OD2	ASP A 54	9	27.076	67.115	86.882	1 00	46.51
	ATOM	4396	N	ALA A 55	U	23.766	64.073	84.032	1.00	27.68
	ATOM	4397	CA	ALA A 55	0	23.445	63.133	82.965	1.00	26.74
	MOTA	4398	С	ALA A 55		22.019	63.171	82.431	1.00	32.35
	ATOM	4399	0	ALA A 55	0	21.745	62.615	81.361	1.00	31.95
15	ATOM	4400	CB	ALA A 55		23.812				
13							61.713	83.372		25.48
	MOTA	4401	N	ILE A 55	1	21.123	63.795	83.192	1.00	28.71
	ATOM	4402	CA	ILE A 55		19.716	63.882	82.832		28.20
	ATOM	4403	С	ILE A 55	1	19.461	64.355	81.411	1.00	32.04
	ATOM	4404	0	ILE A 55	1	18.833	63.679	80.619		31.75
20		,								
20	MOTA	4405	CB	ILE A 55		18.876	64.641	83.868	1.00	30.29
	ATOM	4406	CG1	ILE A 55	1	19.038	63.985	85.226	1.00	31.50
		4407		ILE A 55						
	ATOM					17.391	64.661	83.475		24.75
	ATOM	4408	CD1	ILE A 55	1	18.072	64.561	86.253	1.00	31.62
	ATOM	4409	N	PRO A 55	.2	19.969	65.529	81.099		33.75
25										
23	ATOM	4410	CA	PRO A 55		19.793	66.121	79.796	1.00	32.60
	ATOM	4411	С	PRO A 55	2	20.240	65.224	78.669	1.00	30.34
	ATOM	4412	0	PRO A 55		19.583	65.119	77.622		27.23
	MOTA	4413	CB	PRO A 55	2	20.659	67.383	79.787	1.00	34.45
	MOTA	4414	CG	PRO A 55	2	21.348	67.500	81.139	1.00	38.39
30	ATOM	4415	CD	PRO A 55		20.934	66.296			
50								81.950		34.48
	ATOM	4416	N	LEU A 55	3	21.391	64.616	78.891	-1.00	23.74
	MOTA	4417	CA	LEU A 55	3	21.997	63.727	77.931	1.00	22.72
1, 4	ATOM	4418	С	LEU A 55		21.138	62.522			
								77.670		32.68
	ATOM	4419	0	LEU A 55	3	21.015	62.087	76.523	1.00	35.70
35	MOTA	4420	CB	LEU A 55	3	23.362	63.281	78.439		21.57
	ATOM	4421	CG	LEU A 55						
						24.196	64.496	78.818		24.02
	MOTA	4422	CD1	LEU A 55	3	25.608	64.071	79.174	1.00	19.59
	MOTA	4423	CD2	LEU A 55		24.188	65.479	77.630		18.60
40	ATOM	4424	N	ALA A 55		20.563	61.973	78.754	1.00	30.05
40	ATOM	4425	CA	ALA A 55	4	19.726	60.779	78.669	1.00	27.72
	ATOM	4426	С	ALA A 55		18.432	61.107	77.988		36.03
	ATOM	4427	0	ALA A 55		17.944	60.332	77.163	1.00	37.08
	ATOM	4428	CB	ALA A 55	4	19.475	60.165	80.017	1.00	26.78
	ATOM	4429	N	LEU A 55		17.898	62,283	78.320		
15										29.70
45	MOTA	4430	CA	LEU A 55	5	16.644	62.724	77.720	1.00	28.32
	ATOM	4431	Ç	LEU A 55	55	16.803	62.902	76.229		29.19
	ATOM	4432								
			0	LEU A 55		15.970	62.506	75.385		26.13
	ATOM	4433	CB	LEU A 55	5	16.110	64.027	78.342	1.00	28.26
	ATOM	4434	CG	LEU A 55		15.371	63.814	79.666		32.76
50										
20	ATOM	4435		LEU A 55		15.360	65.118	80.464	1.00	34.66
	ATOM	4436	CD2	LEU A 55	55	13.938	63.334	79.427	1.00	27.50
	ATOM	4437	N	LYS A 55		17.922	63.524	75.950		28.45
	ATOM	4438	CA	LYS A 55		18.325	63.839	74.615	1.00	28.76
2	ATOM	4439	С	LYS A 55	6	18.369	62.591	73.800		35.11
55	ATOM	4440	0	LYS A 55		17.670	62.491			
								72.796		41.80
	ATOM	4441	CB	LYS A 55	96	19.645	64.592	74.599	1.00	31.79
	ATOM	4442	CG	LYS A 55	6	20.101	65.139	73.250		63.55
	ATOM	4443	CD							
				LYS A 55		21.585	65.518	73.254		81.77
	ATOM	4444	CE	LYS A 55	6	22.046	66.270	72.011	1.00	79.68
60	ATOM	4445	NZ	LYS A 55		23.239	65.661	71.401		73.00
	ATOM	4446								
			N	MET A 55		19.154	61.623	74.248		26.96
	MOTA	4447	CA	MET A 55	57	19.305	60.364	73.514	1.00	23.97
	ATOM	4448	С	MET A 55	57	18.033	59.553	73.287		30.96
	ATOM	4449	0	MET A 55). <i>[</i>	17.811	58.907	72.263	1.00	23.24

		ATOM	4450	CB	MET A	557	20.401	59.488	74.104	1.00	24.89
		ATOM	4451	CG	MET A		20.533	58,163	73.368		29.37
			4452	SD	MET A		22.029	57.276	73.864		33.21
		ATOM									
	E	ATOM	4453	CE	MET A		21.939	55.812	72.793		30.16
	5	MOTA	4454	N	ALA A		17.203	59.568	74.287		33.42
		ATOM	4455	CA	ALA A		16.000	58.816	74.194		33.03
		ATOM	4456	С	ALA A		15.042	59.345	73.163	1.00	38.12
		MOTA	4457	0	ALA A	558	14.349	58.568	72.543	1.00	37.09
		MOTA	4458	CB	ALA A	558	15.317	58.780	75.553	1.00	32.89
	10	ATOM	4459	N	THR A	559	14.994	60.665	73.032	1.00	36.76
		ATOM	4460	CA	THR A		14.067	61.326	72.144	1.00	36.43
		MOTA	4461	С	THR A		14.588	61.590	70.794		41.71
		ATOM	4462	ō	THR A		13.788	61.768	69.891		44.66
		ATOM	4463	CB	THR A		13.615	62.705	72.694		43.70
	15	ATOM	4464	OG1	THR A		14.728	63.545	72.957		38.88
	LJ.		4465	CG2	THR A		12.764	62.549	73.942		
		ATOM	4466		GLU A						44.95
		MOTA		N			15.897	61.695	70.674		37.38
,parti		ATOM	4467	CA	GLU A		16.495	62.018	69.395		36.51
Lan.	00	ATOM	4468	С	GLU A		16.652		68.448		40.11
41	20	MOTA	4469	0	GLU A		17.003		67.300		43.23
		ATOM	4470	CB	GLU A		17.799		69.519		38.13
8 ≠£0		ATOM	4471	CG	GLU A		17.653		70.292	1.00	54.29
11 mg 32/5 12 mg 32/5 12 mg 32/5 13 mg 32/5 14 mg 32/5		ATOM	4472	CD	GLU A	560	18.857	65.043	70.127	1.00	78.42
\$40.		ATOM	4473		GLU A		19.960	64.639	69.812	1.00	32.69
5 450 2 450 2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	25	MOTA	4474	OE2	GLU A	560	18.593	66.303	70.380	1.00	85.90
		ATOM	4475	N	GLN A	561	16.425	59.627	68.955	1.00	30.45
		ATOM	4476	CA	GLN A	561	16.467	58.356	68.230	1.00	22.57
碘		ATOM	4477	С	GLN A	561	15.398		68.878	1.00	26.95
B=#%		ATOM	4478	0	GLN A	561	14.978		69.975	1.00	27.79
5 ⁷ 3	30	ATOM	4479	СВ	GLN A		17.829		68.128		20.64
		ATOM	4480	CG	GLN A		18.470		69.491		22.59
		ATOM	4481	CD	GLN A		17.802		70.184		28.22
		MOTA	4482	OE1	GLN A		17.524		71.400		37.44
		ATOM	4483	NE2			17.556		69.419		31.92
l=4.	35	ATOM	4484	N	GLY A		14.888		68.209		26.16
Harrier .		ATOM	4485	CA	GLY A		13.801		68.858		27.83
		ATOM	4486	c c	GLY A		13.932		68.761		41.56
		ATOM	4487	Õ	GLY A		12.936		68.677		45.37
		ATOM	4488	N	ARG A		15.171		68.742		37.40
	40	ATOM	4489	CA	ARG A		15.457		68.689		34.41
		ATOM	4490	C	ARG A				70.109		39.48
		ATOM	4491	Õ	ARG A				71.087		40.29
		ATOM	4492	CB	ARG A				68.284		18.23
		ATOM	4493	CG	ARG A		17.309		68.169		20.07
	45		4404								
	73	ATOM	4494	CD	ARG A		18.779		68.512		25.07
		ATOM	4495	NE	ARG A				68.320		25.66
		ATOM	4496	CZ	ARG A				67.821		26.35
		ATOM	4497		ARG A				67.430		12.96
	50	MOTA	4498		ARG A				67.656		30.31
	20	ATOM	4499	N	MET A				70.239		33.12
		ATOM	4500	CA	MET A				71.526		31.84
		ATOM	4501	С	MET A				72.532		31.42
• *		ATOM	4502	0	MET A				73.744		25.72
	<i></i>	ATOM	4503	CB	MET A				71.365		32.45
	55	ATOM	4504	CG	MET A				70.487		35.78
		ATOM	4505	SD	MET A				70.533		40.85
		ATOM	4506	CE	MET A				69.382		35.87
		ATOM	4507	N	LYS A				71.966		31.68
		ATOM	4508	CA	LYS A	565	16.699	49.041	72.668	1.00	29.04
	60	MOTA	4509	С	LYS A	565	17.283	50.089	73.562		26.36
		ATOM	4510	0	LYS A	565	17.648	49.782	74.673	1.00	21.19
		ATOM	4511	CB	LYS A	565			71.697	1.00	29.06
		MOTA	4512	CG	LYS A	565	18.864	47.715	72.359	1.00	23.89
		ATOM	4513	CD	LYS A	565	19.982	47.355	71.392	1.00	35.75

	MOTA	4514	CE	LYS A	E 6 E	20 706	46 350			
						20.796	46.153	71.842	1.00	36.31
	ATOM	4515	NZ	LYS A	565	22.233	46.311	71.577	1.00	44.91
	ATOM	4516	N	PHE A	566	17.321	51.321	73.073		22.91
	ATOM	4517	CA	PHE A						
5						17.866	52.423	73.833	1.00	24.36
. <i> </i>	ATOM	4518	С	PHE A	566	16.814	53.253	74.571	1.00	30.37
	MOTA	4519	0	PHE A	566	16.882	53.540	75.758		30.52
	ATOM	4520	СВ	PHE A						
						18.622	53.355	72.857	1.00	25.26
	ATOM	4521	CG	PHE A		19.738	52.677	72.088	1.00	24.09
	ATOM	4522	CD1	PHE A	566	20.392	51.559	72.609		
10	ATOM	4523		PHE A						23.51
10						20.165	53.187	70.858	1.00	24.48
	MOTA	4524	CE1	PHE A	566	21.432	50.958	71.900	1.00	23.73
	MOTA	4525	CE2	PHE A	566	21.211	52.620	70.129		24.75
	ATOM	4526	CZ	PHE A						
						21.828	51.491	70.668	1.00	25.20
	ATOM	4527	N	THR A	567	15.860	53.679	73.801	1.00	31.17
15	ATOM	4528	CA	THR A	567	14.783	54.533	74.239		31.74
		4529	C							
	MOTA			THR A		13.985	54.037	75.458	1.00	33.79
	MOTA	4530	0	THR A	567	13.657	54.818	76.373		26.01
	MOTA	4531	CB	THR A	567	13.895	54.892			
								73.017	1.00	36.51
20	MOTA	4532		THR A		14.527	55.844	72.138	1.00	24.12
20	ATOM	4533	CG2	THR A	567	12.522	55.361	73.473		34.94
	ATOM	4534	N	ARG A						
						 13.663	52.726	75.469		30.74
	MOTA	4535	CA	ARG A	568	12.864	52.166	76.545	1.00	26.30
	ATOM	4536	С	ARG A	568	13.486	52.226	77.882		28.61
	MOTA	4537	0	ARG A						
25						12.876	52.667	78.832	1.00	30.84
23	ATOM	4538	CB	ARG A		12.315	50.798	76.251	1.00	18.11
	MOTA	4539	CG	ARG A	568	11.342	50.919	75.088		29.19
	ATOM	4540	CD	ARG A						
						10.550	49.660	74.799	1.00	19.19
	ATOM	4541	NE	ARG A	568	9.707	49.343	75.917	1.00	28.72
	ATOM	4542	CZ	ARG A	568	9.254	48.138	76.133		
30	MOTA	4543		ARG A						32.39
						9.528	47.144	75.291	1.00	29.79
	ATOM	4544	NH2	ARG A		8.507	47.930	77.208	1.00	16.44
	ATOM	4545	N	PRO A	569	14.705	51.774	77.925		28.41
	ATOM	4546	CA	PRO A						
						15.447	51.709	79.154	1.00	28.01
	ATOM	4547	С	PRO A	569	15.890	53.042	79.663	1.00	32.18
35	ATOM	4548	0	PRO A	569	15.974	53.256	80.869		29.25
	ATOM	4549	CB	PRO A		16.607			1.00	23.23
							50.732	78.919		
	MOTA	4550	CG	PRO A		16.330	50.034	77.592	1.00	32.42
	ATOM	4551	CD	PRO A	569	15.234	50.829	76.893		29.82
	ATOM	4552	N	LEU A		16.143	53.949			
40	ATOM	4553						78.741		31.95
40			CA	LEU A		16.560	55.270	79.160	1.00	35.11
	MOTA	4554	С	LEU A	570	15.407	55.962	79.897	1.00	36.24
	ATOM	4555	0	LEU A	570	15.532	56.506	81.028		
	ATOM	4556	СВ							34.02
				LEU A		17.021	56.110	77.932	1.00	37.06
4-	ATOM	4557	CG	LEU A		18.387	55.701	77.343	1.00	41.39
45	MOTA	4558	CD1	LEU A	570	18.678	56.462	76.050		41.06
	ATOM	4559		LEU A						
						19.497	55.984	78.353		37.42
	MOTA	4560	N	PHE A		14.262	55.944	79.211	1.00	30.06
	ATOM	4561	CA	PHE A	571	13.084	56.541	79.758		27.27
	ATOM	4562	С	PHE A						
50						12.813	55.899	81.095		25.94
50	ATOM	4563	0	PHE A		12.399	56.536	82.030	1.00	27.16
	ATOM	4564	CB	PHE A	571	11.888	56 .37 5	78.828		27.60
	ATOM	4565	CG	PHE A		11.546				
							57.616	78.042	1.00	27.70
	MOTA	4566		PHE A		11.193	58.820	78.651	1.00	29.97
	ATOM	4567	CD2	PHE A	571	11.557	57.570	76.651		28.87
5 5	ATOM	4568		PHE A		10.861	59.953			
								77.910		28.24
	ATOM	4569		PHE A		11.233	58 .684	75.886	1.00	30.43
	MOTA	4570	CZ	PHE A	571	10.877	59.875	76.520		29.55
	ATOM	4571	N	LYS A		13.089				
							54.618	81.196		22.77
60	ATOM	4572	CA	LYS A		12.845	53.946	82.468	1.00	25.43
60	ATOM	4573	С	LYS A	572	13.783	54.425	83.561		34.48
	ATOM	4574	0	LYS A		13.351	54.920			
	ATOM	4575	СВ			10 700		84.602		35.11
				LYS A		12.736	52.428	82.392	1.00	26.89
	ATOM	4576	CG	LYS A		11.303	51.911	82.326		44.03
	MOTA	4577	CD	LYS A	572	11.219	50.426	81.922		57.87
					- · ·		20.420	V1.766	. ±.00	31.07

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	MOTA	4578	CE	LYS A 572	10.975	50.204	80.422	1.00 65.25
	ATOM	4579	NZ	LYS A 572	11.535	48.954	79.850	1.00 61.06
	ATOM	4580		ASP A 573	15.074	54.292	83.319	1.00 31.94
	ATOM	4581	CA	ASP A 573	16.032	54.751	84.291	1.00 30.55
5	ATOM	4582	С	ASP A 573	15.684	56.166	84.712	1.00 32.26
	MOTA	4583	0	ASP A 573	15.693	56.453	85.895	1.00 31.85
	MOTA	4584	CB	ASP A 573	17.453	54.788	83.718	1.00 32.87
	MOTA	4585		ASP A 573	18.051	53.443	83.487	1.00 33.43
	ATOM	4586		ASP A 573	17.517	52.422	83.853	1.00 29.11
10	MOTA	4587		ASP A 573	19.206	53.501	82.864	1.00 35.22
	ATOM	4588	N	LEU A 574	15.387	57.071	83.745	1.00 29.50
	ATOM	4589	CA	LEU A 574	15.062	58.461	84.109	1.00 27.65
	ATOM	4590	С	LEU A 574	13.887	58.577	85.075	1.00 32.88
1.5	MOTA	4591	0	LEU A 574	13.864	59.411	85.962	1.00 31.04
15	ATOM	4592	CB	LEU A 574	14.844	59.385	82.909	1.00 26.24
	ATOM	4593	CG	LEU A 574	16.068	59.567 59.922	82.027	1.00 30.41 1.00 28.47
	ATOM	4594 4595		LEU A 574 LEU A 574	15.644 16.974	60.659	80.582 82.604	
14 M	MOTA	4595 4596	N	ALA A 575	12.895	57.723	84.874	1.00 27.06 1.00 32.80
20	ATOM ATOM	4597	CA	ALA A 575	11.709	57.713	85.711	1.00 32.80
₩.#. 40		4598	CA	ALA A 575	12.002	57.140	87.083	1.00 31.11
4.8	MOTA MOTA	4599	0	ALA A 575	11.309	57.362	88.055	1.00 33.71
ha ila	ATOM	4600	CB	ALA A 575	10.631	56.890	85.024	1.00 39.51
#4 340 E #47	ATOM	4601	N	ALA A 576	13.049	56.364	87.170	1.00 30.55
25	ATOM	4602	CA	ALA A 576	13.390	55.778	88.448	1.00 20.33
	ATOM	4603	C	ALA A 576	14.258	56.724	89.266	1.00 26.93
ļ.	ATOM	4604	Ö	ALA A 576	14.444	56.591	90.461	1.00 30.45
**	MOTA	4605	CB	ALA A 576	14.023	54.415	88.245	1.00 20.31
	ATOM	4606	N	PHE A 577	14.787	57.686	88.584	1.00 22.86
30	ATOM	4607	CA	PHE A 577	15.604	58.673	89.194	1.00 22.71
# *** **	ATOM	4608	С	PHE A 577	14.651	59.751	89.673	1.00 32.25
14	ATOM	4609	0	PHE A 577	13.930	60.334	88.863	1.00 34.17
	ATOM	4610	CB	PHE A 577	16.640	59.188	88.154	1.00 22.89
	MOTA	4611	CG	PHE A 577	17.704	60.076	88.741	1.00 23.16
₄ ⊾ 35	MOTA ·	4612	CD1	PHE A 577	17.847	60.231	90.120	1.00 26.60
•	MOTA	4613	CD2	PHE A 577	18.561	60.806	87.914	1.00 23.46
	ATOM	4614		PHE A 577	18.818	61.082	90.661	1.00 27.55
	ATOM	4615	CE2	PHE A 577	19.543	61.657	88.431	1.00 23.88
40	ATOM	4616	CZ	PHE A 577	19.669	61.791	89.813	1.00 23.59
40	ATOM	4617	N	ASP A 578	14.625	60.008	90.990	1.00 29.70
	MOTA	4618	CA	ASP A 578	13.717	61.018	91.533	1.00 28.65
	MOTA	4619	C	ASP A 578	13.862 12.877	62.357	90.881	1.00 28.55 1.00 32.65
	MOTA	4620	O CB	ASP A 578 ASP A 578	13.804	63.004 61.192	90.599 93.055	1.00 32.65
45	ATOM	4621 4622		ASP A 578				
45	ATOM ATOM	4623	CG	ASP A 578	15.153 16.175	61.647	93.550 92.872	1.00 53.21 1.00 51.81
	ATOM	4624		ASP A 578	15.104	62.072	94.796	1.00 64.93
	ATOM	4625	N	LYS A 579	15.104	62.750	90.674	1.00 20.12
	MOTA	4626	CA	LYS A 579	15.470	64.012	90.084	1.00 21.01
50	MOTA	4627	c	LYS A 579	14.934	64.270	88.697	1.00 30.25
	ATOM	4628	Ō	LYS A 579	14.620	65.413	88.368	1.00 35.12
	ATOM	4629	CB	LYS A 579	16.982	64.223	90.104	1.00 24.11
	ATOM	4630	CG	LYS A 579		64.202	91.512	1.00 48.98
	ATOM	4631	CD	LYS A 579	17.252	65.488	92.286	1.00 76.92
55	MOTA	4632	CE	LYS A 579	16.495	65.258	93.588	1.00 87.93
	MOTA	4633	NZ	LYS A 579		64.550	94.611	1.00 89.56
	ATOM	4634	N	SER A 580		63.244	87.857	1.00 28.66
	ATOM	4635	CA	SER A 580		63.437	86.459	1.00 28.56
	ATOM	4636	C	SER A 580		62.829	86.129	1.00 32.95
60	ATOM	4637	0	SER A 580		62.870	84.992	1.00 35.30
	ATOM	4638	СВ	SER A 580		62.774	85.517	1.00 25.69
	MOTA	4639	OG	SER A 580		61.424	85.969	1.00 25.12
	MOTA	4640	N .	HIS A 581		62.230	87.098	1.00 26.81
	ATOM	4641	CA	HIS A 581	11.100	61.595	86.850	1.00 28.26

		T TOOM	1612	~	11TO 3	F 0 1	10.00			
		ATOM	4642	С	HIS A		10.067		86.042	1.00 36.50
		ATOM	4643	0	HIS A		9.644	62.031	84.927	1.00 34.71
		ATOM	4644	CB	HIS A	. 581	10.553	61.047	88.152	1.00 29.76
	_	ATOM	4645	CG	HIS A	581	9.148	60.588	87.968	1.00 35.31
	5	ATOM	4646	ND1	HIS A		8.111		87.899	1.00 38.92
		ATOM	4647		HIS A		8.634		87.891	
		ATOM	4648		HIS A					1.00 36.84
									87.817	1.00 38.85
		MOTA	4649		HIS A		7.280		87.734	1.00 38.13
	10	ATOM	4650	N	ASP A		9.656	63.502	86.639	1.00 35.79
	10	MOTA	4651	CA	ASP A		8.680	64.388	86.064	1.00 34.39
		ATOM	4652	С	ASP A	. 582	9.035	64.807	84.659	1.00 37.82
		MOTA	4653	0	ASP A	582	8.220		83.735	1.00 37.01
		ATOM	4654	CB	ASP A		8.428		87.001	1.00 36.57
		ATOM	4655	CG	ASP A		7.597			
	15	ATOM	4656		ASP A				88.167	1.00 58.09
							6.708		88.070	1.00 63.17
		ATOM	4657		ASP A		7.920		89.279	1.00 73.96
		MOTA	4658	N	GLN A		10.272		84.488	1.00 32.88
CD.	ş	MOTA	4659	CA	GLN A		10.750	65.648	83.169	1.00 29.92
W.		MOTA	4660	С	GLN A		10.690	64.464	82.168	1.00 37.12
क्ष्म झार इन्ह	20	MOTA	4661	0	GLN A	. 583	10.362	64.624	80.990	1.00 37.42
		ATOM	4662	CB	GLN A	583	12.172		83.287	1.00 28.54
ÿ=å.		ATOM	4663	CG	GLN A		12.704		81.929	
		ATOM	4664	CD	GLN A		13.957			1.00 48.12
E##0		ATOM	4665	OE1					82.081	1.00 64.09
55点 35%	25						14.736		83.015	1.00 59.43
	23	ATOM	4666	NE2			14.130		81.201	1.00 55.34
#-# _*		ATOM	4667	N	ALA A		11.009		82.638	1.00 33.22
\$		ATOM	4668	CA	ALA A		10.964	62.062	81.780	1.00 32.22
14		ATOM	4669	С	ALA A	584	9.557	61.841	81.315	1.00 37.45
		MOTA	4670	0	ALA A	584	9.319	61.526	80.152	1.00 40.05
ħ.	30	ATOM	4671	CB	ALA A	584	11.389		82.504	1.00 31.62
Ŋ		ATOM	4672	N	VAL A		8.622		82.261	1.00 31.02
14		ATOM	4673	CA	VAL A		7.217		81.946	
522 MV		ATOM	4674	c	VAL A					1.00 29.16
		ATOM	4675	ō	VAL A		6.647		81.024	1.00 36.53
#=#s	35						5.933		80.052	1.00 36.22
	33	ATOM	4676	CB	VAL A		6.408		83.209	1.00 29.78
		ATOM	4677		VAL A		4.959		82.955	1.00 30.03
		ATOM	4678	CG2	VAL A		6.464	60.085	83.539	1.00 27.82
		ATOM	4679	N	ARG A		7.000	64.123	81.333	1.00 35.76
		ATOM	4680	CA	ARG A	586	6.574	65.242	80.562	1.00 36.20
	40	ATOM	4681	С	ARG A	586	7.146		79.180	1.00 44.65
		ATOM	4682	0	ARG A		6.459		78.197	1.00 48.32
		ATOM	4683	CB	ARG A		7.116		81.208	1.00 38.13
		ATOM	4684	CG	ARG A		6.744		80.518	
		ATOM	4685	CD	ARG A		7.077			1.00 61.01
	45	ATOM	4686		ARG A				81.354	1.00 73.03
		ATOM	4687	CZ			8.491		81.711	1.00 86.05
		ATOM			ARG A		8.961		82.957	1.00 98.46
			4688		ARG A		8.167		84.004	1.00 79.75
		ATOM	4689		ARG A		10.268		83.159	1.00 77.55
	50	ATOM	4690	N	THR A		8.426	64.769	79.110	1.00 39.49
	50	ATOM	4691	CA	THR A	587	9.099	64.646	77.822	1.00 36.80
		ATOM	4692	С	THR A	587	8.387	63.690	76.869	1.00 37.11
		ATOM	4693	0	THR A	587	8.229		75.678	1.00 36.91
		ATOM	4694	CB	THR A		10.634		77.917	1.00 39.40
		ATOM	4695		THR A		11.303			
	55	ATOM	4696		THR A				78.717	1.00 46.27
		ATOM	4697				11.233		76.529	1.00 32.60
				N	TYR A		7.934		77.393	1.00 33.33
		ATOM	4698		TYR A		7.252		76.555	1.00 33.94
	-	ATOM	4699		TYR A		5.890	62.146	76.090	1.00 37.02
	C 0	ATOM	4700		TYR A	588	5.428	61.880	74.988	1.00 41.55
	60	ATOM	4701		TYR A		7.042		77.396	1.00 33.96
		ATOM	4702		TYR A		6.017		76.851	1.00 33.98
		ATOM	4703	CD1	TYR A	588	6.331		75.754	
		ATOM	4704	CD2	TYR A	588	4.758			1.00 35.64
		ATOM	4705	CE1	TYR A	500			77.437	1.00 34.09
			3100	- C13.1	TIN A	500	5.424	57.703	75.251	1.00 34.36

	MOTA	4706	CE2	TYR A	588	3.822	58.378	76.932	1.00 34.05
	ATOM	4707	CZ	TYR A					
						4.162	57.581	75.834	1.00 33.89
	ATOM	4708	OH	TYR A		3.275	56.674	75.322	1.00 23.43
1	ATOM	4709	N	GLN A	589	5.216	62.853	76.959	1.00 25.04
5	MOTA	4710	CA	GLN A	589	3.914	63.339	76.612	1.00 21.41
	ATOM	4711	С	GLN A					
						3.992	64.304	75.481	1.00 28.78
	MOTA	4712	0	GLN A		3.099	64.410	74.678	1.00 31.24
	ATOM	4713	CB	GLN A	589	3.241	63.935	77.832	1.00 21.73
	ATOM	4714	CG	GLN A	589	2.878	62.820	78.827	1.00 22.30
10	MOTA	4715	CD	GLN A		1.695	62.069		
•		4716						78.293	1.00 52.83
	MOTA		OE1			1.511	62.003	77.075	1.00 60.15
	MOTA	4717	NE2			0.864	61.542	79.182	1.00 53.04
	ATOM	4718	N	GLU A	590	5.099	65.001	75.409	1.00 28.36
1 to 1	ATOM	4719	CA	GLU A		5.276	65.966	74.355	1.00 26.87
15	ATOM	4720	C	GLU A					
13						5.840	65.338	73.140	1.00 35.10
	MOTA	4721	0	GLU A	590	6.096	66.059	72.171	1.00 40.28
#FR)	ATOM	4722	CB	GLU A	590	6.323	67.011	74.747	1.00 27.61
	ATOM	4723	CG	GLU A	590	5.846	67.954	75.847	1.00 44.11
H.	ATOM	4724	CD	GLU A					
20						6.981	68.759	76.388	1.00 75.35
	ATOM	4725	OE1			8.120	68.689	75.925	1.00 54.78
je da	ATOM	4726	OE2	GLU A	590	6.609	69.516	77.403	1.00 59.46
·····································	ATOM	4727	N	HIS A	591	6.091	64.031	73.207	1.00 27.57
\$ TEX.	ATOM	4728	CA	HIS A		6.713	63.384		
in:	ATOM	4729	C					72.086	1.00 25.58
35				HIS A		5.928	62.249	71.578	1.00 32.34
25	MOTA	4730	0	HIS A		6.184	61.751	70.496	1.00 38.53
	ATOM	4731	CB	HIS A	591	8.094	62.851	72.487	1.00 26.32
摩	ATOM	4732	CG	HIS A	591	9.219	63.809	72.268	1.00 31.06
∥=#a	ATOM	4733	ND1	HIS A	591	9.630	64.680	73.255	1.00 32.65
30	ATOM	4734		HIS A		9.998	64.032	71.169	1.00 32.03
30	ATOM	4735		HIS A					
						10.635	65.404	72.756	1.00 32.01
C)	ATOM	4736		HIS A		10.884	65.037	71.508	1.00 33.36
	ATOM	4737	N	LYS A		4.978	61.812	72.337	1.00 28.34
	MOTA	4738	CA	LYS A	592	4.254	60.643	71.849	1.00 29.96
-4x	ATOM	4739	С	LYS A	592	3.654	60.692	70.432	1.00 33.41
35	ATOM	4740	0	LYS A	592	3.819	59.769	69.592	1.00 29.05
	ATOM	4741	СВ	LYS A		3.362	59.983		
	ATOM	4742	CG	LYS A				72.888	1.00 32.83
						2.435	60.930	73.615	1.00 31.14
	ATOM	4743	CD	LYS A		1.677	60.203	74.704	1.00 38.97
40	ATOM	4744	CE	LYS A	592	0.253	60.691	74.890	1.00 25.02
40	ATOM	4745	NZ	LYS A	592	-0.157	60.632	76.302	1.00 45.83
	ATOM	4746	N	ALA A	593	2.934	61.782	70.187	1.00 30.97
	ATOM	4747	CA	ALA A		2.260	62.026	68.917	1.00 28.47
	ATOM	4748	C	ALA A		3.169			
	ATOM	4749					61.943	67.703	1.00 32.66
45			0	ALA A		2.775	61.488	66.639	1.00 36.77
45	ATOM	4750	CB	ALA A		1.571	63.379	68.954	1.00 27.35
	MOTA	4751	N	SER A	594	4.384	62.405	67.869	1.00 27.08
	ATOM	4752	CA	SER A	594	5.345	62.417	66.794	1.00 30.04
	ATOM	4753	С	SER A	594	6.185	61.169	66.760	1.00 36.80
	ATOM	4754	0	SER A	594	6.995	60.991	65.848	1.00 37.94
50	ATOM	4755	CB	SER A		6.292	63.596		
	ATOM	4756	OG					66.977	1.00 37.69
				SER A		7.199	63.340	68.043	1.00 54.55
	MOTA	4757	N	MET A		6.015	60.340	67.776	1.00 33.12
	ATOM	4758	CA	MET A		6.794	59.115	67.898	1.00 33.96
	ATOM	4759	С	MET A	595	6.200	57.936	67.125	1.00 40.91
55	ATOM	4760	0	MET A	595	5.019	57.927	66.809	1.00 50.82
	ATOM	4761	CB	MET A		6.716	58.686	69.382	
	ATOM	4762	CG						1.00 34.22
				MET A		7.621	59.371	70.399	1.00 34.61
	ATOM	4763	SD	MET A		7.606	58.440	71.962	1.00 39.24
CO	ATOM	4764	CE	MET A		7.145	59.779	73.084	1.00 36.72
60	MOTA	4765	N	HIS A	596	6.987	56.897	66.886	1.00 26.19
	ATOM	4766	CA	HIS A		6.496	55.657	66.246	1.00 23.19
	ATOM	4767	C	HIS A		5.438	54.964	67.120	1.00 25.21
	ATOM	4768	0 11	HIS A					
						5.621	54.728	68.311	1.00 22.59
	MOTA	4769	CB	HIS A	290	7.657	54.655	66.077	1.00 24.41

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	MOTA	4770	CG	HIS A	596	7.222	53.366	65.493	1.00 30.13
	ATOM	4771	NDI	HIS A	596	7.606	52.995	64.214	1.00 32.86
	ATOM	4772		HIS A		6.421	52,385	66.005	1.00 30.90
		4773		HIS A					
	ATOM					7.047	51.824	63.974	1.00 30.05
5	ATOM	4774		HIS A		6.325	51.441	65.031	1.00 30.20
	ATOM	4775	N	PRO A	597	4.334	54.587	66.512	1.00 27.08
	MOTA	4776	CA	PRO A	597	3.217	53.912	67.173	1.00 26.35
	MOTA	4777	С	PRO A	597	3.513	52.851	68.248	1.00 37.51
	MOTA	4778	0	PRO A		2.979	52.900	69.348	1.00 41.16
10		4779	CB	PRO A				66.076	
10	ATOM					2.334	53.307		1.00 26.17
	A.TOM	4780	CG	PRO A	-	3.140	53.426	64.792	1.00 34.56
	ATOM	4781	CD	PRO A		4.285	54.418	65.050	1.00 30.06
	ATOM	4782	N	VAL A	598	4.311	51.850	67.939	1.00 33.08
	ATOM	4783	CA	VAL A	598	4.585	50.802	68.911	1.00 28.39
15	MOTA	4784	С	VAL A	598	5.444	51.307	70.029	1.00 29.32
	ATOM	4785	Ō	VAL A		5.168	51.096	71.217	1.00 29.13
	MOTA	4786	CB	VAL A		5.196	49.599	68.210	1.00 27.99
	MOTA	4787		VAL A		5.806	48.608	69.187	1.00 26.98
== # <u></u>	MOTA	4788	CG2	VAL A	598	4.144	48.944	67.296	1.00 26.13
20	ATOM	4789	N	THR A	599	6.480	52.021	69.635	1.00 26.10
	ATOM	4790	CA	THR A	599	7.370	52.573	70.631	1.00 26.95
41	ATOM	4791	С	THR A		6.650	53.404	71.669	1.00 30.81
ļ. k	ATOM	4792	0	THR A		6.863	53.327	72.871	
4 140€									1.00 31.33
25	ATOM	4793	CB	THR A		8.413	53.455	69.975	1.00 26.67
25	MOTA	4794	OG1	THR A		9.092	52.725	68.958	1.00 27.92
1J%	MOTA	4795	CG2	THR A	599	9.358	53.884	71.092	1.00 20.69
jet.	MOTA	4796	N	ALA A	600	5.801	54.218	71.135	1.00 26.41
Estate.	MOTA	4797	CA	ALA A	600	4.997	55.111	71.878	1.00 26.39
#	ATOM	4798	C	ALA A		4.176	54.339	72.860	1.00 32.00
30		4799		ALA A					
30	ATOM		0			4.162	54.597	74.057	1.00 35.37
S Table	MOTA	4800	CB	ALA A		4.090	55.774	70.856	1.00 27.56
	ATOM	4801	N	MET A		3.470	53.380	72.332	1.00 26.26
43	ATOM	4802	CA	MET A	601	2.627	52.585	73.167	1.00 26.60
Free Fig.	MOTA	-4803	C	MET A	601	3.439	51.909	74.225	1.00 25.73
35	MOTA	4804	0	MET A		3.099	51.964	75.381	1.00 25.77
3 3	ATOM	4805	СВ	MET A		1.752	51.625	72.353	1.00 30.49
	MOTA	4806	CG	MET A					
						1.024	50.594	73.176	1.00 36.00
	ATOM	4807	SD	MET A		2.043	49.146	73.554	1.00 42.41
40	ATOM	4808	CE	MET A		1.693	48.128	72.111	1.00 37.75
40	ATOM	4809	N	LEU A	602	4.538	51.310	73.848	1.00 21.64
	ATOM	4810	CA	LEU A	602	5.339	50.671	74.873	1.00 22.59
	ATOM	4811	С	LEU A	602	6.010	51.650	75.870	1.00 29.61
	ATOM	4812	0	LEU A		6.137	51.346	77.039	1.00 27.62
	ATOM	4813	ČВ	LEU A		6.418	49.760	74.294	1.00 27.02
15									
45	MOTA	4814	CG	LEU A		5.916	48.529	73.575	1.00 25.78
	MOTA	4815		LEU A		7.021	48.087	72.609	1.00 26.02
	MOTA	4816	CD2	LEU A		5.651	47.445	74.613	1.00 21.01
	ATOM	4817	N	VAL A	603	6.508	52.805	75.445	1.00 27.15
	ATOM	4818	CA	VAL A	603	7.145	53.684	76.413	1.00 26.39
50	ATOM	4819	С	VAL A	603	6.121	54.157	77.438	1.00 32.60
	ATOM	4820	0	VAL A		6.436	54.235	78.621	1.00 35.31
	ATOM	4821	СВ	VAL A		7.917	54.832	75.760	1.00 27.78
								75.700	
	MOTA	4822		VAL A		8.286	55.887	76.774	1.00 24.54
	MOTA	4823		VAL A		9.172	54.286	75.094	1.00 27.29
55	MOTA	4824	N	GLY A		4.878	54.434	76.976	1.00 27.44
	ATOM	4825	CA	GLY A	604	3.759	54.856	77.819	1.00 27.58
	ATOM	4826	С	GLY A		3.418	53.797	78.905	1.00 37.00
	MOTA	4827	Ō	GLY A		3.088	54.102	80.072	1.00 36.56
	ATOM	4828	N	LYS A		3.511	52.522	78.520	1.00 38.50
60	ATOM		CA						
UU.		4829		LYS A		3.250	51.415	79.459	1.00 32.17
	ATOM	4830	C	LYS A		4.312	51.405	80.539	1.00 35.15
	MOTA	4831	0	LYS A		4.040	51.347	81.734	1.00 33.77
	MOTA	4832	CB	LYS A		3.231	50.034	78.782	1.00 33.59
	MOTA	4833	CG	LYS A	605	1.837	49.438	78.576	1.00 42.45

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	MOTA	4834	CD	LYS	Α	605	1.846	48.115	77.815	1.00 60.83
	MOTA	4835	CE	LYS			1.223	46.946	78.578	1.00 86.38
	ATOM	4836	NZ	LYS			2.188	46.179	79.385	1.00 93.05
	ATOM	4837	N	ASP			5.544	51.470	80.056	1.00 32.91
5	ATOM	4838	CA	ASP			6.715	51.510	80.878	1.00 31.82
	ATOM	4839	C	ASP			6.549	52.667	81.833	1.00 36.24
	ATOM	4840	O	ASP			6.652	52.503	83.045	1.00 35.19
	MOTA MOTA	4841 4842	CB CG	ASP ASP			7.983 8.302	51.702 50.525	80.027 79.134	1.00 32.52
10	ATOM	4843		ASP			7.934	49.378	79.344	1.00 40.01 1.00 40.49
. 10	ATOM	4844		ASP			9.038	50.869	78.111	1.00 40.43
	ATOM	4845	N	LEU			6.240	53.833	81.266	1.00 34.45
	ATOM	4846	CA	LEU			6.152	54.972	82.185	1.00 36.03
	ATOM	4847	С	LEU			4.814	55.018	82.968	1.00 42.35
15	MOTA	4848	0	LEU			4.600	55.872	83.824	1.00 41.57
	MOTA	4849	CB	LEU	Α	607	6.321	56.250	81.364	1.00 36.90
	ATOM	4850	CG	LEU	Α	607	7.779	56.490	80.974	1.00 38.75
	MOTA	4851		LEU			7.954	57.746	80.132	1.00 34.34
20	ATOM	4852		LEU			8.695	56.653	82.183	1.00 41.97
₁ 20	ATOM	4853	N	LYS			3.895	54.062	82.586	1.00 45.01
4)	ATOM	4854	CA	LYS			2.576	53.874	83.264	1.00 46.99
į.a.	ATOM	4855	C	LYS			1.625	55.088	83.181	1.00 51.31
11年 12年	ATOM	4856	O	LYS			0.988	55.467	84.151	1.00 51.35
25	ATOM ATOM	4857 4858	CB CG	LYS			2.813 3.331	53.510 52.093	84.750 84.949	1.00 50.83
	ATOM	4859	CD	LYS			4.405	52.019	86.031	1.00 63.57 1.00 77.03
}=4:	ATOM	4860	CE	LYS			5.341	50.825	85.858	1.00 96.40
#	ATOM	4861	NZ	LYS			6.034	50.554	87.117	1.00100.00
	ATOM	4862	N	VAL			1.560	55.724	81.991	1.00 50.28
30	MOTA	4863	CA	VAL	А	609	0.688	56.901	81.852	1.00 50.89
5 m ²	ATOM	4864	С	VAL	Α	609	-0.494	56.660	80.897	1.00 60.23
	ATOM	4865	0	VAL			-1.640	56.952	81.194	1.00 63.02
	ATOM	4866	CB	VAL			1.533	58.091	81.364	1.00 54.72
25	ATOM	4867		VAL			1.996	58.926	82.551	1.00 54.87
35	ATOM ATOM	4868 4869	N	VAL		610	2.744	57.607 56.152	80.605 79.687	1.00 54.46
	ATOM	4870	CA	ASP			-0.177 -1.238	55.949	78.699	1.00 58.84 1.00 99.84
	ATOM	4871	C			610	-2.062	54.695	79.001	1.00100.00
	ATOM	4872	ō			610	-3.247	54.615	78.711	1.00 69.75
40	ATOM	4873	CB			610	-0.594	55.818	77.316	1.00100.00
	ATOM	4874	CG	ASP	Α	610	-0.637	57.161	76.610	1.00 92.61
	ATOM	4875		ASP			-1.449	57.999	77.018	1.00 90.49
	MOTA	4876		ASP			0.134	57.355	75.670	1.00 89.29
15	ATOM		ZN2+		Z	1	17.003	38.803	64.180	1.00 28.37
45	ATOM		YB3+		Y	1	43.011	51.068	98.864	1.00 34.70
	ATOM ATOM		YB3+ YB3+		Y Y	2 3	-13.786 -10.537	56.771 57.860	52.040	0.50 57.25
	ATOM	4881	CG	IMD		1	26.249	42.039	52.381 80.754	0.50 36.57 1.00 28.44
	ATOM	4882		IMD		ī	26.057	42.254	79.400	1.00 28.35
50	MOTA	4883		IMD		1	27.562	41.726	80.902	1.00 17.99
	MOTA	4884		IMD		1	27.201	42.063	78.760	1.00 29.77
	MOTA	4885	NE2	IMD	I	1	28.130	41.745	79.647	1.00 35.02
	ATOM	4886	CB	ACE		1	13.616	12.333	68.475	1.00 59.33
E E	ATOM	4887	CG	ACE		1	12.871	13.331	69.306	1.00 42.98
55	ATOM	4888		ACE		1	12.958	14.536	69.146	1.00 39.66
	ATOM	4889		ACE		1	12.142	12.759	70.236	1.00 47.21
	ATOM	4890	C6	INH			7.422	38.514	70.154	1.00 38.70
	MOTA MOTA	4891 4892	C5 C4	INH			7.571 7.901	39.820 40.062	69.689 68.354	1.00 37.05
60	ATOM	4893		INH			8.091	38.967	67.505	1.00 31.41 1.00 35.48
	ATOM	4894	C2	INH			7.944	37.650	67.949	1.00 33.40
	ATOM	4895		INH			7.611	37.434	69.286	1.00 36.93
	MOTA	4896		INH			8.071	41.463	67.833	1.00 32.28
	MOTA	4897	01	INH			8.288	41.443	66.485	1.00 37.06

		MOTA	4898	C8	INH '		1	9.584	41.740	66.129	1.00 32.34
		ATOM	4899	C9	INH '		1	9.825	42.911	65.416	1.00 31.03
		ATOM	4900		INH '		1	11.127	43.216	65.023	1.00 33.64
	_	ATOM	4901		INH		1	12.194	42.381	65.339	1.00 31.88
	5	ATOM	4902		INH .		1	11.928	41.198	66.028	1.00 31.07
		MOTA	4903		INH		1	10.630	40.858	66.412	1.00 28.70
		MOTA	4904		INH		1	13.587	42.710	64.882	1.00 32.51
		MOTA	4905		INH		1	14.260	41.560	64.121	1.00 34.69
4	10	ATOM	4906		INH		1	15.683	41.849	63.754	1.00 28.88
	10	MOTA	4907	S1	INH		1	16.605	40.755	64.790	1.00 29.16
		ATOM	4908	Nl	INH		1	13.497	40.805	63.099	1.00 30.69
		ATOM	4909	0	HOH !		1	44.463	49.888	77.523	1.00 46.91
		ATOM	4910		HOH !		2	13.469	27.803	78.018	1.00 20.07
	15	ATOM	4911 4912	0	HOH !		3	4.225	69.721	58.393	1.00 27.76
	13	MOTA	4912	0			4	15.603	28.826	61.823	1.00 22.81
		ATOM ATOM	4913	0	HOH I		5 6	22.862	26.624	42.874	1.00 53.05
		ATOM	4914	0			7	8.423	46.452	57.584	1.00 32.22
194 th		ATOM	4916	0	HOH !		8	17.904	46.550	68.524	1.00 31.91
413	20	ATOM	4917	o	HOH 1		9	22.979	45.895	83.716	1.00 39.37
H.	20	ATOM	4918	0	HOH I		10	17.707	39.158	55.643	1.00 25.27
ļ.		ATOM	4919	0	HOH 1		11	12.439 17.367	36.303	59.209	1.00 31.46
# 2500		ATOM	4920	ŏ	HOH 1		12	42.823	62.730	50.320	1.00 37.74
10 mg		ATOM	4921	Ö	HOH 1		13	34.337	52.642	90.552	1.00 53.80
11 (48) 12 (48)	25	ATOM	4922	Õ	HOH I		14	6.726	45.508 27.119	97.419	1.00 57.99
## ##		ATOM	4923	Ö	нон ч		15	-0.093	30.159	48.459 71.746	1.00 62.29
ija An		ATOM	4924	Ö	нон 1		16	-19.673	44.016	58.682	1.00 29.96 1.00 58.64
#		ATOM	4925	Ö	нон 1		17	16.563	26.790	80.837	1.00 38.62
14 14		ATOM	4926	0	нон т		18	10.281	35.677	88.518	1.00 38.02
	30	ATOM	4927	0	нон ч		19	20.973	35.691	44.774	1.00 20.01
ħ.	•	ATOM	4928	0	нон ч		20	0.996	19.571	53.713	1.00 67.39
		ATOM	4929	0	HOH V		21	20.424	37.014	85.845	1.00 39.54
		ATOM	4930	0	HOH I	W.	22	-2.498	35.905	53.781	1.00 51.70
**		ATOM	4931	0	HOH I		23	39.807	49.718	92.595	1.00 37.39
	35	ATOM	4932	0	HOH V	W.	24	16.431	58.267	93.127	1.00 47.45
		ATOM	4933	0	HOH I	W :	25	6.935	45.104	66.012	1.00 18.12
		ATOM	4934	0	HOH I	-	26	40.479	54.713	100.253	1.00 28.72
		ATOM	4935	0	HOH I		27	22.369	40.324	67.919	1.00 46.36
	40	ATOM	4936	0	HOH I		28	37.289	49.457	68.016	1.00 61.37
	40	ATOM	4937	0	нон и		29	2.611	35.015	55.709	1.00 24.45
		ATOM	4938	0	нон ч		30	41.088	62.590	98.644	1.00 65.38
		MOTA	4939	0	нон у		31	17.369	55.024	87.465	1.00 24.22
		ATOM	4940	0	HOH I		32	25.433	20.198	55.692	1.00 44.61
	45	ATOM	4941	0	HOH I		33	3.890	42.770	66.651	1.00 22.34
	73	ATOM ATOM	4942 4943	0	HOH A		34	3.934	63.391	62.592	1.00 60.69
		ATOM	4944	0	HOH I		35 36	22.280	41.610	86.289	1.00 74.20
		ATOM	4945	0	HOH I		36 37	22.631 33.442	46.401 20.227	90.078	1.00 47.44
		ATOM	4946	Ö	нон ч			39.834	28.974	64.569	1.00 55.41
	50	ATOM	4947	Ō	нон т		39	35.232	47.140	75.602 54.186	1.00 41.72
		ATOM	4948	Ö	нон т		40	36.003	57.784	57.893	1.00 37.08 1.00 43.05
		ATOM	4949	0	нон т		41	37.216	27.438	74.564	1.00 43.03
		MOTA	4950	0	нон ч		42	17.770	67.012	77.183	1.00 45.78
		ATOM	4951	0	нон и		43	5.341	31.286	78.127	1.00 45.78
	55	ATOM	4952	0	HOH V		44	33.535	32.503	52.063	1.00 56.13
		MOTA	4953	0	нон и		45	25.477	33.146	44.610	1.00 65.43
		ATOM	4954	0	нон т		46	16.235	37.438	52.628	1.00 32.10
		MOTA	4955	0	нон и		47	28.791	14.101	63.316	1.00 46.67
	<i>-</i>	MOTA	4956	0	HOH V		48	10.230	24.992	86.967	1.00 38.63
	60	MOTA	4957	0	HOH V		49	30.821	38.856	79.630	1.00 40.44
		MOTA	4958	0	HOH V		50	12.621	37.226	62.944	1.00 26.70
		ATOM	4959	Ο.	HOH V	N :	51		30.609	66.612	1.00 33.55
		ATOM	4960	0	HOH A		52	34.459	28.696	64.242	1.00 51.01
		MOTA	4961	0	HOH I	N .	53	34.969	62.270	91.179	1.00 68.20

	7.000	40.00								
	MOTA	4962	0	HOH W	54	33.631	30.717	62.396	1.00	41.64
	ATOM	4963	0	HOH W	55					50.99
	MOTA	4964	0	HOH W	56					69.23
	ATOM	4965	0	HOH W	57					81.00
5	MOTA	4966	0	HOH W	58					38.96
	ATOM	4967	0	HOH W	59					40.28
	ATOM	4968	0	HOH W	60					21.71
	ATOM	4969	ō	HOH W	61					37.69
	ATOM	4970	Ō	HOH W	62					
10	ATOM	4971	Ö	HOH W	63					41.05
	ATOM	4972	ŏ	HOH W	64					28.51
	ATOM	4973	ō	HOH W	65					89.05
	ATOM	4974	Ö	HOH W	66					38.43
	ATOM	4975	ő	HOH W	67					55.25
15	ATOM	4976	Ö	HOH W	68					92.26
	ATOM	4977	Ö	HOH W	69					59.25
	ATOM	4978	ŏ	HOH W	70					52.24
	ATOM	4979	0	HOH W						77.81
[3	ATOM	4980	0	HOH W	71					36.83
20	ATOM	4981			72					32.24
4.)	ATOM	4982	0	HOH W	73					40.73
-4.			0	HOH W	74					38.90
	ATOM	4983	0	HOH W	75					54.53
100g 200g 100g 200g	ATOM	4984	0	HOH W	76					55.38
25	ATOM	4985	0	HOH W	77				1.00	40.09
23	ATOM	4986	0	HOH W	78					29.78
}=# ₄	MOTA	4987	0	HOH W	79					35.92
	MOTA	4988	0	HOH W	80	19.320				33.36
# 8 s	MOTA	4989	0	HOH W	81	28.815			1.00	59.19
h	ATOM	4990	0	HOH W	82			73.585	1.00	17.81
1.30	ATOM	4991	0	HOH W	83	23.802			1.00	25.19
n.	ATOM	4992	0	HOH W	84	42.241		99.896	1.00	15.88
La.	ATOM	4993	0	HOH W	85	3.751		58.842	1.00	24.97
	ATOM	4994	0	HOH W	86	-7.009	40.341		1.00	25.39
	ATOM	4995	0	HOH W	87	11.735	58.910	68.155	1.00	39.70
35	MOTA	4996	0	HOH W	88	13.986	52.835	42.224	1.00	50.91
	ATOM	4997	0	HOH W	89	1.452		69.459	1.00	35.03
	ATOM	4998	0	HOH W	90	-1.938	55.310		1.00	28.10
	ATOM	4999	0	HOH W	91	13.801		52.600	1.00	38.65
40	ATOM	5000	0	HOH W	92	21.594	47.218	79.203	1.00	30.31
40	ATOM	5001	0	HOH W	93	10.639	58.632	90.827	1.00	43.78
	ATOM	5002	0	HOH W	94	33.335	53.550		1.00	37.04
	ATOM	5003	0	HOH W	95	-1.984	28.738	60.212	1.00	31.56
	ATOM	5004	0	HOH W	96	-4.958	51.055	59.250	1.00	34.00
15	ATOM	5005	0	HOH W	97	17.610		51.503	1.00	28.27
45	MOTA	5006	0	HOH W	98	10.686		67.565		37.68
	ATOM	5007	0	HOH W	99	20.567	43.859		1.00	41.57
	ATOM	5008	0	HOH W		7.013		69.109	1.00	28.72
	ATOM	5009	0	HOH W		10.097		78.477		35.68
50	ATOM	5010	0	HOH W		10.849	31.404	53.014	1.00	32.22
50	MOTA	5011	0	HOH W		42.381		94.728		36.00
	MOTA	5012	0	HOH W		17.234		54.082		33.65
	ATOM	5013	0	HOH W		26 .9 02		81.989		34.70
	MOTA	5014	0	HOH W		-14.313	49.559	56.204		54.36
E E	ATOM	5015	0	HOH W		41.646	57.501	101.015		68.12
55	ATOM	5016	0	HOH W		26.759	43.000	47.219		32.69
	MOTA	5017	0	HOH W		16.624		46.545		38.64
	MOTA	5018	0	HOH W		26.159		75.230		24.77
	MOTA	5019	0	HOH W		2.101		67.006		31.50
~~	ATOM	5020	0	HOH W	112	38.114		87.451		44.06
60	MOTA	5021	0	HOH W	113	13.211		61.356		33.81
	ATOM	5022	0	HOH W		-3.064		40.673		37.92
	MOTA	5023	0	HOH W	115	15.007		69.488		28.23
	MOTA	5024	0	HOH W		27.101		80.518		41.24
	ATOM	5025	0	HOH W	117	11.870		43.174	1.00	40.85

		ATOM	5026	0	HOH W 118	-13.844	25.597	58.258	1.00 53.75
		ATOM	5027	ō	HOH W 119	2.929	41.135	59.858	1.00 36.49
		ATOM	5028	Ō	HOH W 120	24.890	45.490	82.167	1.00 41.65
		MOTA	5029	Ō	HOH W 121	36.062	59.335	75.090	1.00 38.82
	5	ATOM	5030	ō	HOH W 122	-10.715	32.037	61.699	1.00 78.82
	_	ATOM	5031	ō	HOH W 123	-2.646	25.492	60.812	1.00 48.40
		ATOM	5032	ō	HOH W 124	-8.948	46.831	63.556	1.00 48.06
		ATOM	5033	ō	HOH W 125	-17.843	39.367	36.020	1.00 35.80
		ATOM	5034	Ö	HOH W 126	2.218	57.766	62.253	1.00 44.61
	10	ATOM	5035	ŏ	HOH W 127	10.736	62,766	64.366	1.00 55.84
	10	ATOM	5036	Ö	HOH W 128	0.884	35.562	63.963	1.00 44.14
		ATOM	5037	ŏ	HOH W 129	19.165	59.557	60.644	1.00 47.82
		ATOM	5038	Ö	HOH W 130	1.546	27.875	68.443	1.00 39.69
		ATOM	5039	ŏ	HOH W 131	5.497	26.285	76.668	1.00 44.47
	15	ATOM	5040	ŏ	HOH W 132	14.505	36.538	88.996	1.00 40.00
	1.5	MOTA	5040	Ö	HOH W 133	8.534	28.713	88.519	1.00 46.55
			5042	ő	HOH W 134	6.125	45.267	77.959	1.00 45.57
		ATOM ATOM	5042	Ö	HOH W 135	26.016	18.543	78.878	1.00 43.57
17		ATOM	5043	Ö	HOH W 136	33.880	23.025	70.739	1.00 31.03
· 支班(20	1.2	5045		HOH W 137	19.230	26.073	49.998	1.00 40.93
		MOTA	5045		HOH W 137	41.563	41.085	77.326	
12 116	and M.	ATOM	5047	0	HOH W 139	39.187	63.067	75.380	1.00 43.14 1.00 56.52
##\		ATOM		0	HOH W 140	26.878		67.203	
144 <u>8</u> ens		ATOM	5048 5049	0	HOH W 141		54.491 62.189		1.00 42.14
सम्बद्धाः इसरः	25	ATOM		0	HOH W 141	22.988 25.190		74.174	1.00 48.31 1.00 67.16
ŲŤ.	23	ATOM	5050	0	HOH W 142		62.803	71.067	
### ###		ATOM	5051	0		18.598	45.126	81.949	1.00 53.80
H= est		ATOM	5052	0	HOH W 144	19.782	53.129	90.556	1.00 48.73
學		ATOM	5053	0	HOH W 145	21.735	48.367	86.454	1.00 40.39
jad.	20	ATOM	5054	0	HOH W 146	25.707	57.012	93.476	1.00 53.61
ST. III	30	MOTA	5055	0	HOH W 147	22.832	62.085	93.149	1.00 46.02
7.		MOTA	5056	0	HOH W 148	25.725	67.203	89.990	1.00 75.23
25 42 5 44		MOTA	5057	0	HOH W 149	10.773	53.653	85.697	1.00 50.65
क्षेत्र स्तुर्थ इंक सहर		ATOM	5058	0	HOH W 150	4.221	58.449	86.608	1.00 49.23
	25	MOTA	5059	0	HOH W 151	7.790	72.096	84.410	1.00 51.10
l-k	35	ATOM	5060	0	HOH W 152	2.387	58.282	67.835	1.00 33.29
		ATOM	5061	0	HOH W 153	0.921	49.551	69.095	1.00 59.60
		ATOM	5062	0	HOH W 154	8.722	45.171	71.561	1.00 46.56
		ATOM ATOM	5063 5064	0	HOH W 155 HOH W 156	6.422 15.936	47.947 56.908	81.081 55.129	1.00 57.56 1.00 43.33
	40	ATOM	5065	0	HOH W 157	3.032	19.635	62.453	1.00 43.33
	70	MOTA	5066	Ö	HOH W 158	-4.228	58.058	47.057	1.00 39.66
		MOTA	5067	o	HOH W 159	1.197	41.002	78.942	1.00 57.22
		ATOM	5068	Ö	HOH W 160	1.259	43.651	68.100	1.00 37.22
		ATOM	5069	Ö	HOH W 161	25.799	64.833	56.690	1.00 37.94
	45	ATOM	5070	ő	HOH W 162	-11.853	45.054	45.070	1.00 38.38
	73	ATOM	5070	ő	HOH W 163	40.159	31.033	78.548	1.00 38.36
		ATOM	5072	Ö	HOH W 164	21.477	20.377	79.349	1.00 75.30
		ATOM	5073	Ö	HOH W 165	26.347	44.558	72.803	1.00 33.30
		ATOM	5074	ő	HOH W 166	16.446	61.207	59.687	1.00 39.70
	50	MOTA	5075	ō	HOH W 167	27.695	64.216	82.410	1.00 44.71
	-	ATOM	5076	õ	HOH W 168	-2.998	57.511	34.738	1.00 45.35
		MOTA	5077	ŏ	HOH W 169	6.608	51.527	60.826	1.00 39.48
		ATOM	5078	ŏ	HOH W 170	31.104	28.934	81.337	1.00 43.19
		ATOM	5079	Ö	HOH W 171	10.135	28.233	45.533	1.00 41.24
	55	ATOM	5080	Ö	HOH W 172	8.201	43.960	75.322	1.00 37.71
		ATOM	5081	Ö	HOH W 172	13.799	66.601	85.597	1.00 37.71
		ATOM	5082	0	HOH W 174	16.664	53.670	65.006	1.00 34.74
		ATOM	5083	0	HOH W 174	18.301	47.296	43.793	1.00 45.84
		ATOM	5084	0	HOH W 176	11.717	61.868	52.648	1.00 45.84
	60	ATOM	5085	0	HOH W 177	29.516	23.822	76.838	1.00 54.93
	. 55	ATOM	5086	Ö	HOH W 178	39.940	60.509	78.535	1.00 31.30
		ATOM	5087	Ö	HOH W 179	-1.803	44.974	37.278	1.00 46.33
		ATOM	5088	Ö	HOH W 179	7.343	47.305	65.468	1.00 32.36
		ATOM	5089	0	HOH W 181	17.912	15.338	81.793	1.00 47.27
		AIOH	2003	J	11011 # 101	11.512	10.000	01.193	1.00 30.00

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ATOM 5090 0 HOH W 182 -4.631 55.917 82.183 1.00 65.36 ATOM 5092 0 HOH W 184 -1.834 36.784 71.040 1.00 45.10 ATOM 5093 0 HOH W 185 -1.834 36.784 71.040 1.00 45.10 ATOM 5093 0 HOH W 186 -4.519 34.633 71.838 1.00 43.95 36.74 71.661 1.00 46.99 ATOM 5096 0 HOH W 186 -4.518 66.554 71.661 1.00 46.99 ATOM 5096 0 HOH W 188 31.770 43.526 51.410 1.00 58.02 ATOM 5096 0 HOH W 189 5.471 43.861 38.891 1.00 49.96 34.70M 5098 0 HOH W 199 5.471 43.861 38.891 1.00 49.96 34.70M 5090 0 HOH W 191 31.12 26.03 70.484 1.00 60.09 ATOM 5090 0 HOH W 191 31.12 26.03 70.484 1.00 60.09 ATOM 5100 0 HOH W 192 30.914 43.017 70.613 1.00 73.23 ATOM 5102 0 HOH W 193 0.00 43.00 39.914 1.00 49.96 34.70M 5102 0 HOH W 195 12.39 59.92 62.698 1.00 53.75 34.70M 5102 0 HOH W 195 12.39 59.92 62.698 1.00 53.75 34.70M 5106 0 HOH W 196 11.149 17.504 78.264 1.00 60.09 34.70M 5106 0 HOH W 197 -4.284 31.93 60.991 1.00 47.10 34.70M 3106 0 HOH W 198 29.888 35.624 82.772 1.00 52.16 34.70M 5106 0 HOH W 200 -8.529 51.475 47.745 1.00 61.00 34.70M 5106 0 HOH W 200 -8.529 51.475 47.745 1.00 61.00 34.70M 5108 0 HOH W 200 -8.529 51.475 47.745 1.00 61.00 34.70M 5108 0 HOH W 200 -8.529 51.475 47.745 1.00 61.00 34.70M 5108 0 HOH W 200 -8.529 51.475 47.745 1.00 61.00 34.70M 5108 0 HOH W 200 -8.529 51.475 47.745 1.00 61.00 34.70M 5108 0 HOH W 200 -8.529 51.475 47.745 1.00 61.00 34.70M 5108 0 HOH W 200 -8.529 51.475 47.745 1.00 61.00 34.70M 5108 0 HOH W 200 -8.529 51.475 61.00 41.00 41.00 41.00 41.00 41.00 41.00 41.00 41.00 41.00 41.00 41.00									
ATOM 5091		ATOM	5090	0	HOH W 182	-4.631	55.917	82.183	1.00 65.36
ATOM 5093 0 HOH W 184 -1.834 36.784 71.040 1.00 45.10 ATOM 5093 0 HOH W 185 -4.519 34.633 71.838 1.00 43.9 5 ATOM 5095 0 HOH W 186 4.518 66.554 71.661 1.00 46.99 ATOM 5095 0 HOH W 187 2.774 37.503 61.490 1.00 45.8 6.02 ATOM 5095 0 HOH W 189 31.770 43.526 51.410 1.00 58.02 ATOM 5096 0 HOH W 189 31.770 43.526 51.410 1.00 58.02 ATOM 5096 0 HOH W 199 11.934 58.219 70.811 1.00 49.96 ATOM 5099 0 HOH W 199 11.934 58.219 70.811 1.00 49.96 ATOM 5090 0 HOH W 191 31.112 26.203 70.484 1.00 60.09 ATOM 5100 0 HOH W 191 31.012 49.00 30.914 43.017 70.613 1.00 73.23 ATOM 5100 0 HOH W 193 0.914 43.017 70.613 1.00 73.23 ATOM 5102 0 HOH W 194 48.247 56.159 86.370 1.00 60.09 ATOM 5102 0 HOH W 195 12.359 55.992 62.698 1.00 53.7 51.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 60.09 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.00 39.714 1.00 65.00 40.00 39.00 39.00 39.714 1.00 65.00 40.00 39.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.714 1.00 65.00 40.00 39.00 39.7									
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## ATOM 5108 O HOH W 200 -8.529 51.475 47.745 1.00 61.00 ## ATOM 5109 O HOH W 201 -15.572 53.338 52.008 1.00 72.42 ## ATOM 5110 O HOH W 202 24.319 38.590 87.128 1.00 50.03 ## ATOM 5111 O HOH W 203 25.366 70.670 82.839 1.00 49.01 ## ATOM 5112 O HOH W 204 18.531 27.749 86.236 1.00 49.01 ## ATOM 5113 O HOH W 205 21.694 20.030 81.796 1.00 49.04 ## ATOM 5115 O HOH W 207 22.012 40.217 90.228 1.00 42.29 ## ATOM 5116 O HOH W 207 22.012 40.217 90.228 1.00 56.50 ## ATOM 5117 O HOH W 209 21.019 68.958 84.382 1.00 56.50 ## ATOM 5118 O HOH W 210 -7.134 33.015 71.591 1.00 56.31 ## ATOM 5120 O HOH W 211 40.843 44.050 89.284 1.00 56.50 ## ATOM 5120 O HOH W 212 20.374 14.856 56.642 1.00 50.07 ## ATOM 5120 O HOH W 212 20.374 14.856 56.642 1.00 59.15 ## ATOM 5120 O HOH W 213 12.723 46.277 73.748 1.00 59.15 ## ATOM 5123 O HOH W 215 -2.433 36.012 80.232 1.00 54.12 ## ATOM 5125 O HOH W 216 5.257 25.271 55.914 1.00 53.23 ## ATOM 5126 O HOH W 217 13.354 64.403 53.662 1.00 53.23 ## ATOM 5126 O HOH W 219 14.139 47.479 76.123 1.00 79.04 ## ATOM 5128 O HOH W 229 29.563 50.769 1.00 48.10 ## ATOM 5130 O HOH W 221 32.979 51.667 96.624 1.00 51.30 ## ATOM 5131 O HOH W 222 14.677 45.948 71.756 1.00 55.94 ## ATOM 5131 O HOH W 221 32.979 51.667 96.624 1.00 55.94 ## ATOM 5133 O HOH W 221 32.979 51.667 96.624 1.00 55.94 ## ATOM 5131 O HOH W 223 33.890 24.505 58.094 1.00 43.65 ## ATOM 5133 O HOH W 224 17.853 9.19 65.660 1.00 35.63 ## ATOM 5133 O HOH W 224 17.853 9.19 65.660 1.00 35.63 ## ATOM 5134 O HOH W 237 33.843 36.070 55.8									
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ATOM 5112 O HOH W 204 18.531 27.749 86.236 1.00 48.64 25 ATOM 5113 O HOH W 205 21.694 20.030 81.796 1.00 49.04 ATOM 5115 O HOH W 206 23.953 47.993 67.580 1.00 42.39 ATOM 5116 O HOH W 207 22.012 40.217 90.228 1.00 42.29 ATOM 5117 O HOH W 208 16.197 45.094 43.427 1.00 48.00 ATOM 5118 O HOH W 209 21.019 68.985 84.382 1.00 56.50 ATOM 5119 O HOH W 210 -7.134 33.015 71.591 1.00 56.31 ATOM 5120 O HOH W 211 40.843 44.050 89.284 1.00 43.07 ATOM 5121 O HOH W 212 20.374 14.856 56.642 1.00 50.07 ATOM 5122 O HOH W 213 12.723 46.277 73.748 1.00 59.15 ATOM 5123 O HOH W 214 8.956 43.704 58.706 1.00 45.56 ATOM 5124 O HOH W 216 5.257 25.271 55.914 1.00 54.12 ATOM 5125 O HOH W 217 13.354 64.403 53.862 1.00 47.27 ATOM 5126 O HOH W 219 14.139 47.479 76.123 1.00 79.04 ATOM 5127 O HOH W 219 14.139 47.479 76.123 1.00 79.04 ATOM 5128 O HOH W 220 0.829 29.563 50.769 1.00 48.10 ATOM 5131 O HOH W 221 12.979 51.667 96.624 1.00 52.31 ATOM 5131 O HOH W 223 13.890 24.505 58.094 1.00 53.34 ATOM 5133 O HOH W 223 13.890 24.505 58.094 1.00 53.34 ATOM 5134 O HOH W 225 17.953 95.19 65.560 1.00 55.94 ATOM 5135 O HOH W 227 4.932 48.808 63.354 1.00 42.45 ATOM 5134 O HOH W 228 18.933 59.070 55.899 1.00 50.38 ATOM 5135 O HOH W 228 18.933 59.070 55.899 1.00 50.38 ATOM 5136 O HOH W 228 18.933 59.070 55.899 1.00 50.38 ATOM 5137 O HOH W 231 27.565 65.998 75.153 1.00 73.11 ATOM 5130 O HOH W 228 18.933 59.070 55.899 1.00 50.39 ATOM 5131 O HOH W 231 27.565 65.998 75.153 1.00 73.11 ATOM 5134 O HOH W 231 27.565 65.998 75.153 1.00 73.11 ATOM 5134 O HOH W 233 27.128 39.012 68.497 1.00 40.77 ATOM 5141 O HOH W 233 40.706 52.468 74.641 1.00 51.60 ATOM 5142 O HOH W 234 12.699 65.312 58.091 1.00 50.79 ATOM 5143 O HOH W 235 9.121 17.615 59.271 1.00 66.79 ATOM 5144 O HOH W 236 17.931 36.565 8.091 1.00 54.77 ATOM 5145 O HOH W 242 18.399 33.843 66.007 52.576 1.00 61.60 ATOM 5140 O HOH W 241 8.399 33.843 6.007 52.576 1.00 61.60 ATOM 5140 O HOH W 241 8.399 33.843 6.007 52.576 1.00 61.60 ATOM 5145 O HOH W 244 18.399 33.818 71.442 1.00 68.05	13			0			38.590	87.128	1.00 50.03
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ATOM 5113 O HOH W 205 23.953 47.993 67.580 1.00 49.04 ATOM 5115 O HOH W 207 22.012 40.217 90.228 1.00 42.29 ATOM 5116 O HOH W 207 22.012 40.217 90.228 1.00 42.29 ATOM 5117 O HOH W 208 16.197 45.094 43.427 1.00 48.00 ATOM 5118 O HOH W 209 21.019 68.985 84.382 1.00 56.50 ATOM 5119 O HOH W 211 40.843 44.050 89.284 1.00 43.07 ATOM 5120 O HOH W 212 20.374 14.856 56.642 1.00 50.07 ATOM 5121 O HOH W 213 12.723 46.277 73.748 1.00 45.56 ATOM 5122 O HOH W 214 8.956 43.704 58.706 1.00 45.56 ATOM 5123 O HOH W 215 -2.433 36.012 80.232 1.00 54.12 ATOM 5124 O HOH W 216 5.257 25.271 55.914 1.00 53.17 ATOM 5125 O HOH W 217 13.354 64.03 53.862 1.00 47.27 ATOM 5126 O HOH W 218 30.477 42.517 67.472 1.00 48.10 ATOM 5127 O HOH W 219 14.139 47.479 76.123 1.00 79.04 40 ATOM 5129 O HOH W 221 32.979 51.667 96.624 1.00 51.30 ATOM 5130 O HOH W 221 32.979 51.667 96.624 1.00 55.31 ATOM 5131 O HOH W 222 14.677 45.948 71.756 1.00 55.31 ATOM 5132 O HOH W 222 14.677 45.948 71.756 1.00 55.31 ATOM 5133 O HOH W 222 17.853 9.519 65.560 1.00 55.94 ATOM 5133 O HOH W 222 17.853 9.519 65.560 1.00 55.94 ATOM 5134 O HOH W 225 37.794 31.473 62.305 1.00 50.38 ATOM 5133 O HOH W 225 37.794 31.473 62.305 1.00 55.03 ATOM 5134 O HOH W 226 29.206 50.335 62.673 1.00 45.43 ATOM 5137 O HOH W 227 4.932 48.808 63.354 1.00 42.45 ATOM 5138 O HOH W 228 18.933 59.010 68.497 1.00 45.43 ATOM 5139 O HOH W 221 17.853 9.519 65.560 1.00 55.94 ATOM 5131 O HOH W 223 12.7565 65.098 75.153 1.00 75.03 ATOM 5134 O HOH W 231 27.565 65.098 75.153 1.00 75.63 ATOM 5134 O HOH W 233 27.128 39.012 68.497 1.00 51.60 ATOM 5140 O HOH W 233 40.706 52.468 74.641 1.00 51.60 ATOM 5141 O HOH W 233 33.843 36.0707 52.576 1.00 61.60 ATOM 5141 O HOH W 233 33.843 36.0707 52.576 1.00 61.60 ATOM 5143 O HOH W 239 44.272 44.279 81.461 1.00 54.07 ATOM 5140 O HOH W 239 44.272 44.279 81.461 1.00 54.07 ATOM 5141 O HOH W 239 44.272 44.279 81.461 1.00 69.21 ATOM 5140 O HOH W 241 8.39 33.818 71.442 1.00 66.05 ATOM 51510 O HOH W 244 16.173 45.408 46.636 1.00 20.00	\$14k	ATOM	5112	0	HOH W 204	18.531	27.749	86.236	1.00 48.64
ATOM 5115 O HOH W 207 ATOM 5116 O HOH W 208 ATOM 5117 O HOH W 209 ATOM 5117 O HOH W 209 ATOM 5118 O HOH W 210 ATOM 5118 O HOH W 210 ATOM 5118 O HOH W 211 ATOM 5120 O HOH W 211 ATOM 5121 O HOH W 212 20.374 14.856 56.642 1.00 59.07 ATOM 5121 O HOH W 213 ATOM 5122 O HOH W 213 ATOM 5122 O HOH W 214 ATOM 5124 O HOH W 215 ATOM 5125 O HOH W 216 ATOM 5126 O HOH W 217 ATOM 5126 O HOH W 217 ATOM 5127 O HOH W 218 ATOM 5126 O HOH W 218 ATOM 5127 O HOH W 219 ATOM 5128 O HOH W 219 ATOM 5129 O HOH W 220 ATOM 5130 O HOH W 221 ATOM 5130 O HOH W 221 ATOM 5131 O HOH W 222 ATOM 5131 O HOH W 223 ATOM 5131 O HOH W 224 ATOM 5131 O HOH W 225 ATOM 5131 O HOH W 227 ATOM 5131 O HOH W 228 ATOM 5131 O HOH W 229 ATOM 5133 O HOH W 227 ATOM 5134 O HOH W 228 ATOM 5135 O HOH W 227 ATOM 5136 O HOH W 227 ATOM 5137 O HOH W 228 ATOM 5138 O HOH W 229 ATOM 5139 O HOH W 220 ATOM 5130 O HOH W 220 ATOM 5131 O HOH W 221 ATOM 5131 O HOH W 223 ATOM 5131 O HOH W 224 ATOM 5133 O HOH W 224 ATOM 5134 O HOH W 225 ATOM 5135 O HOH W 227 ATOM 5136 O HOH W 227 ATOM 5137 O HOH W 230 ATOM 5138 O HOH W 227 ATOM 5136 O HOH W 230 ATOM 5137 O HOH W 230 ATOM 5137 O HOH W 230 ATOM 5138 O HOH W 231 ATOM 5136 O HOH W 231 ATOM 5137 O HOH W 231 ATOM 5136 O HOH W 231 ATOM 5137 O HOH W 231 ATOM 5136 O HOH W 231 ATOM 5137 O HOH W 231 ATOM 5136 O HOH W 231 ATOM 5137 O HOH W 231 ATOM 5136 O HOH W 233 ATOM 5137 O HOH W 233 ATOM 5138 O HOH W 233 ATOM 5137 O HOH W 233 ATOM 5136 O HOH W 233 ATOM 5141 O HOH W 233 ATOM 5141 O HOH W 234 ATOM 5147 O HOH W 237 ATOM 5146 O HOH W 238 ATOM 5147 O HOH W 238 ATOM 5147 O HOH W 238 ATOM 5148 O HOH W 240 ATOM 5149 O HOH W 241 ATOM 5140 O HOH W 242 ATOM 5147 O HOH W 238 ATOM 5146 O HOH W 240 ATOM 5147 O HOH W 241 ATOM 5148 O HOH W 240 ATOM 5150 O HOH W 241 ATOM 5150 O	अर्थुं का इ.स.	ATOM	5113	0	HOH W 205	21.694	20.030		1.00 49.04
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ATOM 5116 O HOH W 208 16.197 45.094 43.427 1.00 48.00 ATOM 5117 O HOH W 209 21.019 68.985 84.382 1.00 56.50 ATOM 5118 O HOH W 210 -7.134 33.015 71.591 1.00 56.31 ATOM 5120 O HOH W 211 40.843 44.050 89.284 1.00 43.07 ATOM 5121 O HOH W 213 12.723 46.277 73.748 1.00 59.15 ATOM 5122 O HOH W 213 12.723 46.277 73.748 1.00 59.15 ATOM 5122 O HOH W 214 8.956 43.704 58.206 1.00 45.56 ATOM 5122 O HOH W 216 5.257 25.271 55.914 1.00 53.23 ATOM 5124 O HOH W 216 5.257 25.271 55.914 1.00 53.23 ATOM 5125 O HOH W 217 13.354 64.403 53.862 1.00 47.27 ATOM 5127 O HOH W 219 14.139 47.479 76.123 1.00 79.04 ATOM 5128 O HOH W 221 14.139 47.479 76.123 1.00 79.04 ATOM 5128 O HOH W 221 14.139 47.479 76.123 1.00 79.04 ATOM 5128 O HOH W 221 32.979 51.667 96.624 1.00 51.30 ATOM 5130 O HOH W 222 14.677 45.948 71.756 1.00 52.31 ATOM 5130 O HOH W 222 14.677 45.948 71.756 1.00 52.31 ATOM 5133 O HOH W 222 14.677 45.948 71.756 1.00 52.31 ATOM 5133 O HOH W 222 14.677 45.948 71.756 1.00 52.31 ATOM 5133 O HOH W 222 14.677 45.948 71.756 1.00 52.31 ATOM 5133 O HOH W 222 14.677 45.948 71.756 1.00 52.31 ATOM 5133 O HOH W 222 14.687 95.660 50.335 62.673 1.00 43.65 ATOM 5133 O HOH W 222 14.808 863.354 1.00 42.45 ATOM 5133 O HOH W 222 14.808 863.354 1.00 42.45 ATOM 5133 O HOH W 222 13.849 18.833 83.641 1.00 55.89 ATOM 5133 O HOH W 229 13.849 18.833 83.641 1.00 55.89 ATOM 5133 O HOH W 229 13.849 18.833 83.641 1.00 55.63 ATOM 5133 O HOH W 229 13.849 18.833 83.641 1.00 55.63 ATOM 5134 O HOH W 230 25.919 46.022 68.076 1.00 55.63 ATOM 5140 O HOH W 231 27.565 65.098 75.153 1.00 73.11 ATOM 5140 O HOH W 233 40.706 52.468 74.641 1.00 51.60 ATOM 5141 O HOH W 233 40.706 52.468 74.641 1.00 51.98 ATOM 5141 O HOH W 233 40.706 52.468 74.641 1.00 51.98 ATOM 5140 O HOH W 233 40.706 52.468 74.641 1.00 51.98 ATOM 5141 O HOH W 233 40.706 52.468 74.641 1.00 51.98 ATOM 5141 O HOH W 233 40.706 52.468 74.641 1.00 51.98 ATOM 5140 O HOH W 234 41.642 42.79 81.6461 1.00 69.21 ATOM 5146 O HOH W 238 42.642 42.79 81.6461 1.00 69.21 ATOM 5146 O HOH W 238 42.642 42.79 81.6461 1.00 69.21 AT		ATOM		0	HOH W 207	22.012	40.217		
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ATOM 5150 O HOH W 242 1.051 31.947 69.204 1.00 52.88 ATOM 5151 O HOH W 243 44.255 51.162 96.650 1.00 20.00 ATOM 5152 O HOH W 244 16.173 45.408 46.636 1.00 20.00									1.00 54.01
ATOM 5151 O HOH W 243 44.255 51.162 96.650 1.00 20.00 ATOM 5152 O HOH W 244 16.173 45.408 46.636 1.00 20.00	60								
ATOM 5152 O HOH W 244 16.173 45.408 46.636 1.00 20.00				0			31.947	69.204	1.00 52.88
ATOM 5152 O HOH W 244 16.173 45.408 46.636 1.00 20.00		MOTA	5151	0	HOH W 243	44.255	51.162	96.650	
ATOM 5153 O HOH W 245 41.130 50.734 97.991 1.00 20.00	• 1 A	the second second		0				46.636	1.00 20.00
		MOTA	5153	0	HOH W 245	41.130	50.734	97.991	1.00 20.00

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ATOM ATOM ATOM ATOM ATOM	5154 5155 5156 5157 5158	0 0 0	HOH W 246 HOH W 247 HOH W 248 HOH W 249 HOH W 250	-17.107 24.078 -12.250 35.804	27.146 46.307	54.728 79.123 61.593	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00
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5

CLAIMS

- 1. An isolated protein comprising at least a subsequence of the amino acid sequence of LTA₄ hydrolase, which exhibits a three-dimensional form essentially as disclosed in Table 9 by the parameters defining atom 1 to atom 4876, said subsequence being capable of participating in the control of the an enzymatic pathway, such as the leukotriene cascade, or a functionally equivalent part, derivative or conformational analogue thereof.
- 2. A protein according to claim 1, which comprises an enzymatically active site defined in the following table:

	Left wall	Right wall
1		Lys608, Asp606, Lys605, Lys354, Thr355
2	Phe356, Phe362	Gln544, Asp573, Lys572, Arg568
3	Val376	Lys565, Arg540, Leu507
4	Ser380, Ser352, Glu348	Pro569
5	Tyr378, Glu348	Arg563, Glu533, Phe536, Arg537, Tyr267
6	Tyr383, Phe314, Glu318, Glu384, Arg326	
7	Gly268, Gly269, Met270	His295, Asn341, Phe340
8	Ser288, His497	Glu325, Asn291

- 3. A protein according to claim 2, which is an enzyme having a metallohydrolase activity capable of participating in the regulation of enzyme activities in biochemical pathways, wherein said enzymes have structures similar to the ones defined in claim 2.
- 4. A protein according to claim 1, which comprises an enzymatically active site defined by the following amino acids: Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; Glu296; His299; Glu318; Tyr378; Tyr383; Arg563; Lys565.
- A protein according to claim 1, which comprises an enzymatically active site defined by the following amino acids: Gln136; Ala137; Tyr267; Gly268; Gly269;
 Met270; Glu271; Val292; His295; Glu296; His299; Trp315; Glu318; Val322:

- Phe362; Val367; Leu369; Pro374; Asp375; Ile372; Ala377; Pro382; Tyr378; Tyr383; Arg563; Lys565.
- 6. A compound which is substantially complementary to a protein according to any one of claims 1-5.
- 7. A compound according to claim 6, which is substantially complementary to an enzymatically active site of said protein and which is capable of specifically inhibiting said enzymatic activity.
 - 8. A compound according to claim 7, which is an inhibitor of a metallohydrolase enzyme.
 - 9. An isolated complex, which is comprised of a protein according to claim 1-5 and a complementary compound according to any one of claims 6-8, wherein the three-dimensional structure of LTA₄ hydrolase is essentially as disclosed in Table 9 by the parameters defining atom 1- atom 4876, or a functionally equivalent part, derivative or conformational analogue of such a complex.
 - 10. A complex according to claim 9, wherein the protein complexed with LTA₄ hydrolase is selected from the group which consists of bestatin, thiolamine or hydroxamic acid, or a functionally equivalent part, derivative or conformational analogue of such a complex.
 - 11. Use of the parameters of a protein according to any one of claims 1-5, a compound according to any one of claims 6-8 or a complex according to claim 9 or 10 in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry.
 - 12. Use according to claim 11, wherein said parameters are selected from the parameters disclosed in Table 9 defining atom 1- atom 4876.
- 25 13. Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of disorders involving acute and chronic inflammatory and/or allergic symtoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS).
- 30 14. Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer.

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- 15. Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax.
- 16. A method for screening LTA₄ hydrolase analogues that mimic at least a part of the three dimensional structure of the LTA₄ hydrolase molecule as defined by the parameters shown in Table 9 for atom 1 to atom 4876, which comprises the steps of
- (a) producing a multiplicity of analogue structures of LTA₄ hydrolase and
- (b) selecting an analogue structure, wherein the three-dimensional configuration and spatial arrangement of one or more enzymatically active sites and/or binding sites of said LTA₄ hydrolase remain substantially preserved.
- 17. A method according to claim 16, wherein an analogue exhibiting an enzymatic activity, such as an epoxide hydrolase and/or aminopeptidase activity, is selected.
- 18. A method according to claim 16 or 17, wherein an enzymatic inhibitor complementary to the amino acids defined in any one of claims 3, 4 or 5 is screened for.
- 19. An analogue obtainable by the method according to any one of claims 16-18.
- 20. An analogue according to claim 19, which exhibits an increased catalytic activity when compared to the naturally occurring form of LTA₄ hydrolase, such as defined in Table 9 by parameters of atom 1 to atom 4876.
- 21. A method for screening LTA₄ hydrolase binding compounds complementary to a region of LTA₄ hydrolase, preferably an enzymatically active site thereof, which comprises the steps of
 - (a) producing a multiplicity of possible complementary structures and
 - (b) selecting a structure, wherein the three-dimensional configuration and spatial arrangement of regions involved in binding to LTA₄ hydrolase remain substantially preserved, which selection is based on the three-dimensional structure of LTA₄ hydrolase, and/or LTA₄ hydrolase complexed to an inhibitor thereof, in a form adopted thereof in nature, such as defined in Table 9.
 - 22. A method according to claim 21, wherein a general metallohydrolase inhibitor is selected, which is capable of inhibiting an enzyme belonging to the M1 family.

- 23. A method according to claim 21, wherein an inhibitor of the epoxide hydrolase activity and/or aminopeptidase activity of LTA₄ hydrolase or of LTC₄ synthases is selected.
- 24. A method according to claim 21, wherein a compound capable of antagonizing LTB₄ receptor binding of a cell is selected.
- 25. A compound obtainable by the method according to any one of claims 21-24.
- 26. A method of engineering a protein, which method comprises the steps of
- -identification of a suitable set of mutations based on the structure of LTA₄ hydrolase;
- -generation of a library of genes which contains the suitable sequence variations;
- -selection of clones encoding the LTA₄ hydrolase analogues with a desired activity function;
 - wherein said desired activity is the capability of efficiently producing an organic compound of interest.
- 27. A method according to claim 26, wherein the specified property is the suicidal mode of action of LTA₄ hydrolase.
- 28. A process for the purification of a protein according to any one of claims 1-3 or obtained according to claim 26 or 27, which purification includes hydroxyapatite-based chromatography and a subsequent anion exchange chromatography.
- 29. A process for the crystallisation of an LTA₄ hydrolase, an analogue or a derivative thereof, wherein said crystallisation is performed with the addition of a ytterbium salt as an additive, such as an ytterbium chloride.
 - 30. A protein obtained by the method according to any one of claims 27-29.
 - 31. A protein according to claim 30, which is present in an essentially pure form.
- 25 32. An isolated nucleic acid encoding a protein according to claim 30 or 31.
 - 33. A nucleic acid capable of specifically hybridising to a the nucleic acid according to claim 32.
 - 34. Use of a protein, which is a genetically modified LTA₄ hydrolase, according to claim 30 or 31 in the preparation of LTB₄ or other metabolites in the leukotriene cascade.

- 35. A protein according to any one of claims 6-8, 25, 30 or 31 for use as a medicament.
- 36. Use of a protein according to any one of claims 6-8, 25, 30 or 31 in the manufacture of a medicament for the treatment and/or prevention of acute and chronic inflammatory and/or allergic disorders, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis and chronic obstructive pulmonary disease (COPD); neoplasias and/or cancer; or disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax.
- 37. Use of a protein according to any one of claims 6-8, 25, 30 or 31, in the manufacture of a medicament for the treatment and/or prevention of an anti-inflammatory and/or anti-allergenic disorder, such as bronchial asthma, allergic rhinitis, conjunctivitis etc.
- 38. Use of a protein according to any one of claims 6-8, 25, 30 or 31 in the manufacture of a medicament for the treatment and/or prevention of infection caused be human immunodeficiency virus (HIV).

Figure 1

Figure 2

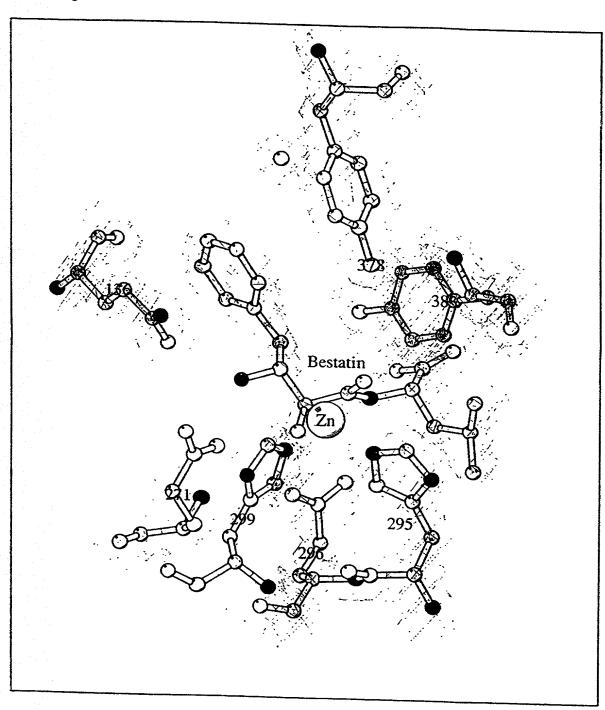
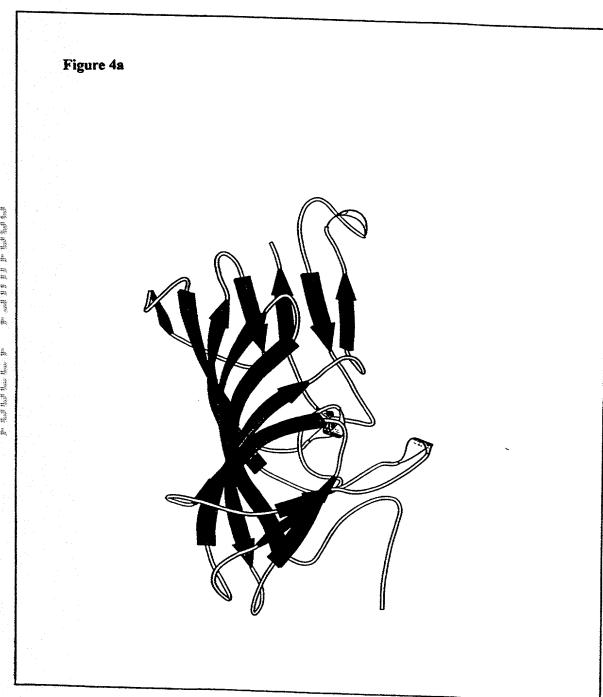
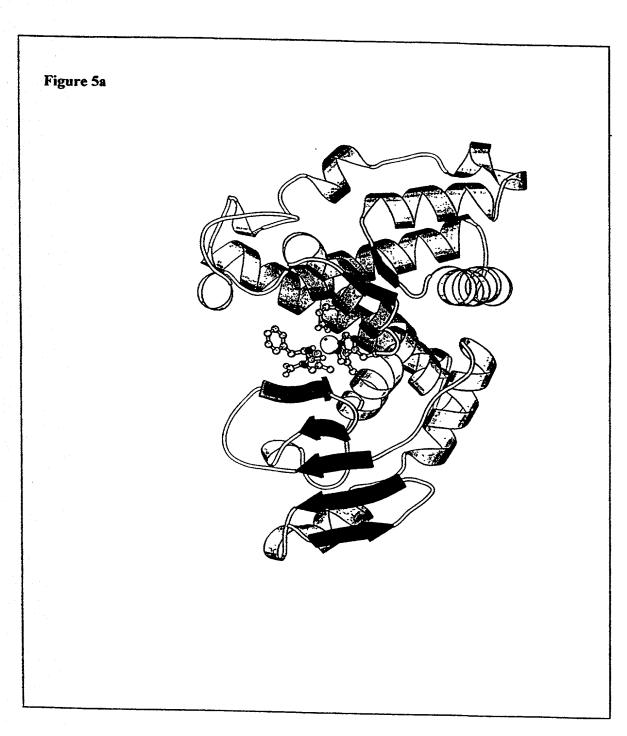


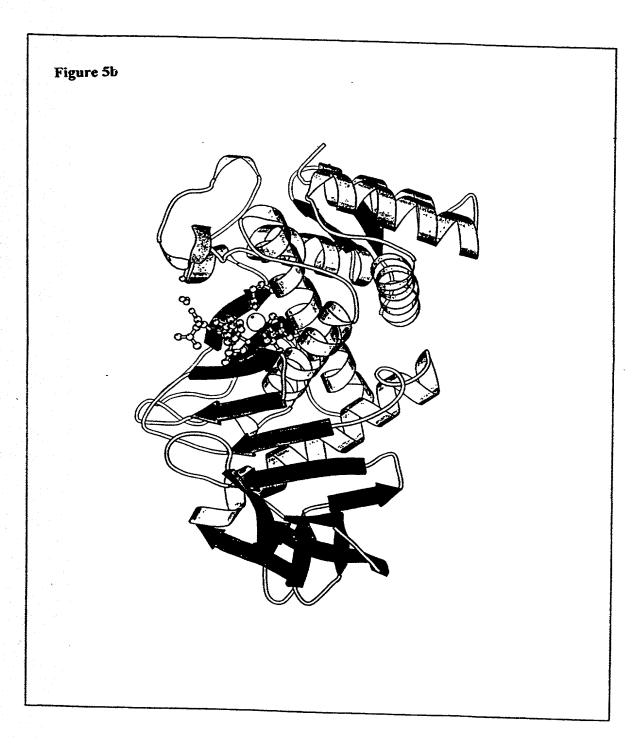
Figure 3











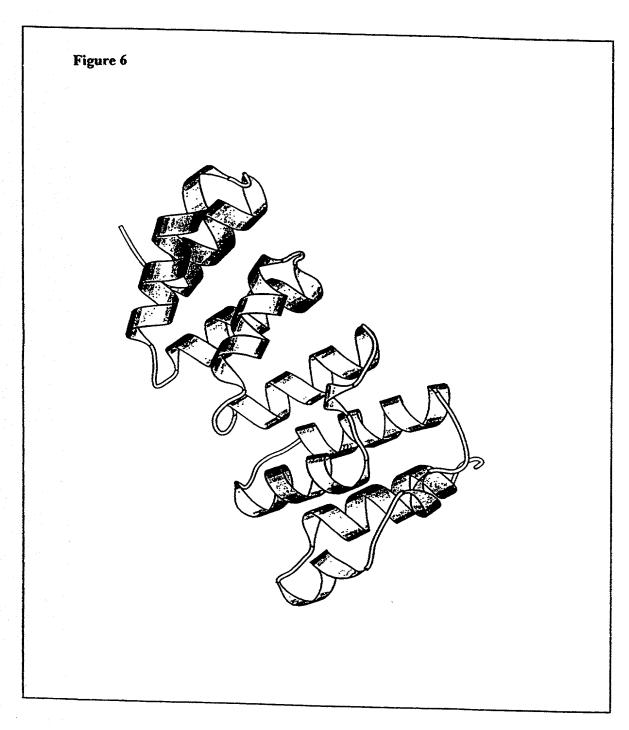
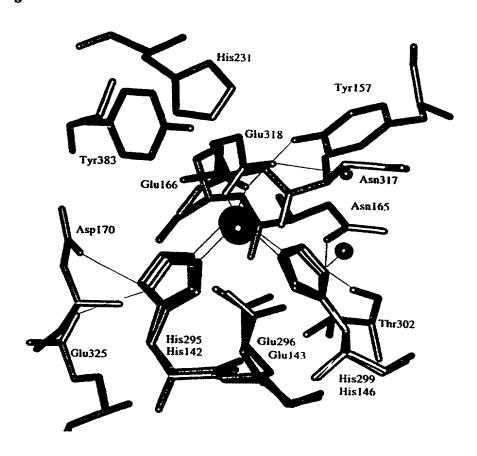


Figure 7



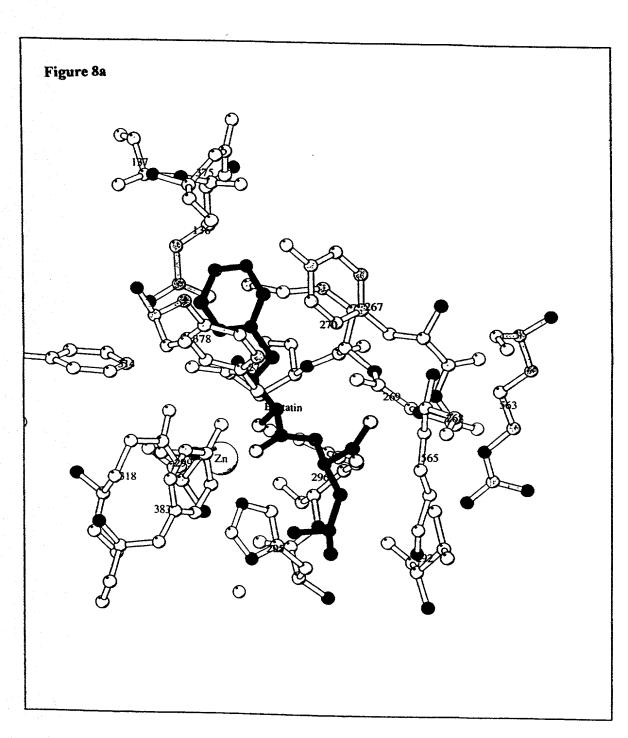
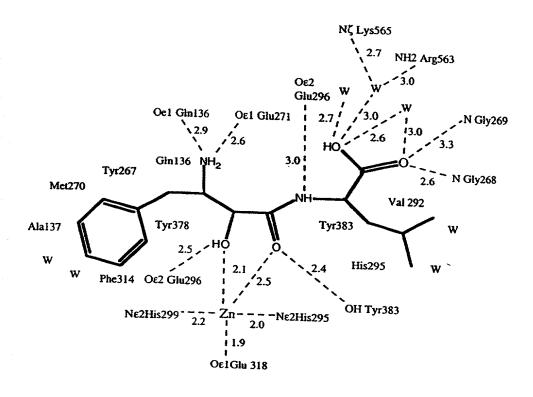


Figure 8b



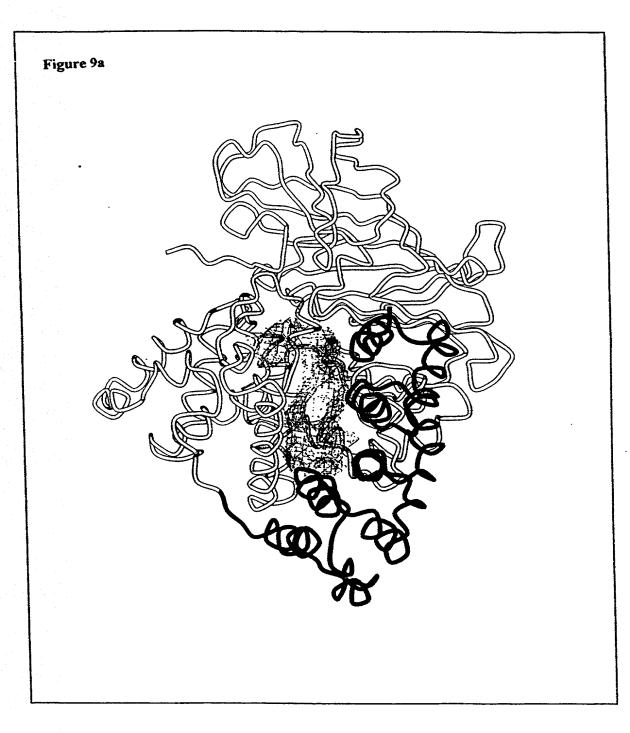
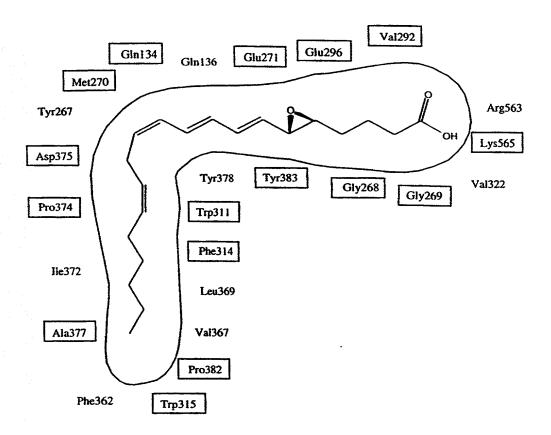


Figure 9b



(Check one):

DECLARATION, PETITION AND POWER OF ATTORNEY FOR PATENT APPLICATION

☑ Declaration Submitted with Initial Filing
☐ Declaration Submitted after Initial Filing
As a below named inventor, I hereby declare that:
My residence, post office address and citizenship are as stated below next to my name,
I believe I am the original, first and sole inventor (if only one name is listed below) or an original, first and joint inventor (if plural names are listed below) of the subject matter which is claimed and for which a patent is sought on the invention entitled:
DRUG DESIGN BASED ON THE STRUCTURE OF LTA4 HYDROLASE
the specification of which (check one):
is attached hereto.
OR
was filed on 28 February 2000 as PCT International Application Number
PCT/SE00/00384
and was amended by PCT Article 19 Amendment on (if applicable),
and was amended by PCT Article 34 Amendment on(if applicable).
I acknowledge the duty to disclose to the Office all information known to me to be material to patentability as defined in Title 37, Code of Federal Regulations, §1.56.
I hereby state that I have reviewed and understood the contents of the above-identified specification, including the claims, as amended by any amendment referred to above.

PRIORITY CLAIM

(Check one):							
□ no such applic	ations have be	en filed.					
such application	ns have been	filed as follow	ws				
1) FOREIGN PRIOR States Code, §119(a)-(d §365(a) of any PCT inte United States of Americ application for patent or before that of the applic	or §365(b) of rnational applica, listed below inventor's cert	any foreign ap cation which d and have also ificate or any I	plication lesignation identif PCT interpretation	on(s) for patent of ted at least one of fied below, by cl	or inventor country oth necking the	's certific er than the box, any	ate or ie foreign
Prior Foreign	Country	Foreign Fil	ling	Priority	Certifie		1
Application Number(s)		Date (mm,dd,yy	777	Not Claimed	Attac Yes	hed No	
9900722-1	SE	26 February	1999			×	!
		(26.02.99	<u>)</u>				
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☐ Additional foreign a 2) PROVISIONAL PR Code §119(e) of any Un	CORITY CLA	IM : I hereby	√ claim	the benefit unde	·		
Provisional Application	Number(s)	11	Filing I	Date (mm/dd/yy	w)		
60/122,110	14uiiioCi(s)			ruary 1999 (26.			
Additional provision hereto. 3) U.S./PCT PRIORIT §120 of any United State United States of America pplication is not discloprovided by the first part disclose information who of Federal Regulations, and the national or PCT	EY CLAIM: I es application of a, listed below sed in the prior agraph of Title ich is known to §1.56 which be international fi	hereby claim to \$365(c) of an and, insofar as United States 35, United States are to be mate came available ling date of the	the benny PCT sthe su or PCT ates Coerial to between is applications.	efit under Title of international applicational applicational applicational applications are filling data ication.	35, United oplication of the oplication is owledge the defined in the of the price	States Co designating claims of in the man de duty to Title 37, ior applic	ode, ng the this nner Code ation
U.S. Parent Application Number	PCT Parent 1	1		Filing Date I/yyyy)	Parent I	Patent Nui	mber
				··	(5 %)		
☐ Additional U.S. or P sheet attached hereto.	CT internationa	al application r	numbei	rs are listed on a	supplemer	ntal priori	ty

POWER OF ATTORNEY:

As a named inventor, I hereby appoint the following attorneys and/or agents to prosecute this application and transact all business in the Patent and Trademark Office connected therewith.

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Thomas V. Smurzynski	Reg. No. 24,798	Jeremiah Lynch	Reg. No. 17,425
Ralph A. Loren	Reg. No. 29,325	David J. Rikkers	Reg. No. 43,882
Giulio A. DeConti, Jr.	Reg. No. 31,503	Maria C. Laccotripe	Limited Recognition
Ann Lamport Hammitte	Reg. No. 34,858	-	Under 37 C.F.R. § 10.9(b)
Elizabeth A. Hanley	Reg. No. 33,505	Debra J. Milasincic	Reg. No. 46,931
Amy E. Mandragouras	Reg. No . 36,20 7	David R. Burns	Reg. No. 46,590
Anthony A. Laurentano	Reg. No. 38,220	Sean D. Detweiler	Reg. No. 42,482
Kevin J. Canning	Reg. No. 35,470	Peter S. Stecher	Reg. No. 47,259
Jane E. Remillard	Reg. No. 38,872	Cynthia L. Kanik	Reg. No. 37,320
Peter C. Lauro	Reg. No. 32,360	Theodore R. West	Reg. No. 47,202
DeAnn F. Smith	Reg. No. 36,683	Shayne Y. Huff	Reg. No. 44,784
Jeanne M. DiGiorgio	Reg. No. 41,710	·	

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Elizabeth A. Hanley, Esq. Lahive & Cockfield, LLP, 28 State Street, Boston, Massachusetts 02109, United States of America

Direct Telephone Calls to: (name and telephone number)

Elizabeth A. Hanley, Esq., (617) 227-7400

Wherefore I petition that letters patent be granted to me for the invention or discovery described and claimed in the attached specification and claims, and hereby subscribe my name to said specification and claims and to the foregoing declaration, power of attorney, and this petition.

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

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Inventor's signature Engli Hologan	Date 2001 -11 - 05
Residence Valhallavägen 145, SE-115 31 Stockholm,	C+
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Residence	2_1
Gruvbacken 2, SE-116 34 Stockholm, SWEDEN 🧪	ŻV
Citizenship	4
SE	
Post Office Address (if different)	

Full name of third inventor

THUNISSEN, Marjolein

Inventor's signature

Date

Zoo (- ((- 0)

Citizenship

NL

Post Office Address (if different)

1-4

M. 1

JC03 Rec'd PCT/PTO 2 7 AUG 2001

PCT/SE00/00384

WO 00/50577

SEQUENCE LISTING

1

<110> Haeggström et al., Jesper <120> DRUG DESIGN BASED ON THE STRUCTURE OF LTA4 HYDROLASE <130> 54660 <140> <141> <160>1 <170> PatentIn Ver. 2.1 <210>1 <211>611 <212> PRT <213> HUMAN <220> <223> AMINO ACID SEQUENCE OF HUMAN LEUKOTRIENE A4 **HYDROLASE** <400> 1 Met Pro Glu Ile Val Asp Thr Cys Ser Leu Ala Ser Pro Ala Ser Val 10 Cys Arg Thr Lys His Leu His Leu Arg Cys Ser Val Asp Phe Thr Arg Arg Thr Leu Thr Gly Thr Ala Ala Leu Thr Val Gln Ser Gln Glu Asp 40 Asn Leu Arg Ser Leu Val Leu Asp. Thr Lys Asp Leu Thr Ile Glu Lys Val Val Ile Asn Gly Gln Glu Val Lys Tyr Ala Leu Gly Glu Arg Gln 75 80 Ser Tyr Lys Gly Ser Pro Met Glu Ile Ser Leu Pro Ile Ala Leu Ser Lys Asn Gln Glu Ile Val Ile Glu Ile Ser Phe Glu Thr Ser Pro Lys 100 105 110 Ser Ser Ala Leu Gln Trp Leu Thr Pro Glu Gln Thr Ser Gly Lys Glu 120 125 His Pro Tyr Leu Phe Ser Gln Cys Gln Ala Ile His Cys Arg Ala Ile 135 140 Leu Pro Cys Gln Asp Thr Pro Ser Val Lys Leu Thr Tyr Thr Ala Glu 150 155 Val Ser Val Pro Lys Glu Leu Val Ala Leu Met Ser Ala Ile Arg Asp

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PHURET ROS 20 DEC 2011

H'S

SEQUENCE LISTING

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Val Lys Thr Phe Gly Glu Thr His Pro Phe Thr Lys Leu Val Val Asp 355 360 365

Leu Thr Asp Ile Asp Pro Asp Val Ala Tyr Ser Ser Val Pro Tyr Glu 370 375 380

Lys Gly Phe Ala Leu Leu Phe Tyr Leu Glu Gln Leu Leu Gly Gly Pro 385 390 395 400

Glu Ile Phe Leu Gly Phe Leu Lys Ala Tyr Val Glu Lys Phe Ser Tyr 405 410 415

Lys Ser Ile Thr Thr Asp Asp Trp Lys Asp Phe Leu Tyr Ser Tyr Phe 420 425 430

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